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Generalised CP symmetry in modular-invariant models of flavour

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ABSTRACT: The formalism of combined finite modular and generalised CP (gCP) symmetries for theories of flavour is developed. The corresponding consistency conditions for the two symmetry transformations acting on the modulus τ and on the matter fields are derived. The implications of gCP symmetry in theories of flavour based on modular invariance described by finite modular groups are illustrated with the example of a modular S_4 model of lepton flavour. Due to the addition of the gCP symmetry, viable modular models turn out to be more constrained, with the modulus τ being the only source of CP violation.

KEYWORDS: Beyond Standard Model, CP violation, Neutrino Physics

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1 Introduction

Explaining the flavour structures of quarks and leptons remains to be one of the fundamental problems in particle physics. We still do not know the absolute values of neutrino masses, as well as whether CP symmetry is violated in the lepton sector. However, the observed pattern of neutrino mixing with two large and one small (but non-zero) angles suggests that a non-Abelian discrete flavour symmetry can be at work (see [1–4] for reviews).

In the bottom-up discrete symmetry approach to lepton flavour, some of the neutrino mixing angles and the Dirac CP violation (CPV) phase δ are generically predicted to be correlated with each other, since all of them are expressed in terms of few free parameters. At the same time, the Majorana phases [5], present in the neutrino mixing matrix if neutrinos are Majorana particles, remain unconstrained. In order to reduce the number of free parameters, the discrete flavour symmetry can be combined with the so-called generalised CP (gCP) symmetry [6, 7]. Such models have more predictive power and allow, in particular, for prediction of the Majorana phases. The implications of combining the gCP symmetry with a flavour symmetry have been extensively studied for many discrete groups, including A_4 [7, 8], T' [9], S_4 [6, 10–15] and A_5 [16–19] (see also [20]).

The conventional bottom-up discrete symmetry approach to lepton flavour has certain drawbacks. Within this approach specific models need to be constructed to obtain predictions for neutrino masses. A flavour symmetry in these models is typically spontaneously broken by vacuum expectation values (VEVs) of scalar flavon fields. Usually, a relatively large number of these fields with a rather complicated potential possessing additional shaping symmetries to achieve the correct vacuum alignment is needed. Possible higher-dimensional operators may affect model predictions, and thus, have to be taken into account.

In view of that, a new approach, in which modular invariance plays the role of flavour symmetry, has been put forward in ref. [21]. The main feature of this approach is that the Yukawa couplings and fermion mass matrices in the Lagrangian of the theory arise from modular forms which depend on the value of a single complex scalar field τ , called the modulus. In addition, both the couplings and fields transform under a finite modular group Γ_N . Once τ acquires a VEV, the Yukawa couplings and the form of the mass matrices get fixed, and a certain flavour structure arises. For $N \leq 5$, the finite modular groups are isomorphic to permutation groups (see, e.g., [22]) used to build models of lepton and quark flavours. Until now models based on the finite modular groups $\Gamma_2 \simeq S_3$ [23, 24], $\Gamma_3 \simeq A_4$ [21, 23–29], $\Gamma_4 \simeq S_4$ [30, 31] and $\Gamma_5 \simeq A_5$ [32, 33] have been constructed in the literature. In a top-down approach, the interplay of flavour and modular symmetries has recently been considered in the context of string theory in refs. [34–36].

In the present work, we study the implications of combining the gCP symmetry with modular invariance in the construction of models of flavour. It is expected that combining the two symmetries in a model of flavour will lead to a reduction of the number of free parameters, and thus to an increased predictive power of the model. The article is organised as follows. In section 2, we summarise key features of combining gCP symmetry with a discrete non-Abelian group and briefly describe the modular symmetry approach to flavour. Then, in section 3, requiring consistency between CP and modular symmetries, we derive the action of CP on i) the modulus, ii) superfields and iii) multiplets of modular forms. After that, in section 4, we discuss implications for the charged lepton and neutrino mass matrices, and determine the values of the modulus which allow for CP conservation. In section 5, we give an example of a viable model invariant under both the modular and CP symmetries. Finally, we conclude in section 6.

2 Framework

2.1 Generalised CP symmetry combined with a flavour symmetry

Consider a supersymmetric (SUSY) theory¹ with a flavour symmetry described by a non-Abelian discrete group G_f . A chiral superfield $\psi(x)$ in a generic irreducible representation (irrep) **r** of G_f transforms under the action of G_f as

$$\psi(x) \xrightarrow{g} \rho_{\mathbf{r}}(g) \psi(x), \quad g \in G_f,$$
(2.1)

where $\rho_{\mathbf{r}}(g)$ is the unitary representation matrix for the element g in the irrep \mathbf{r} . A theory which is also invariant under CP symmetry has to remain unchanged under the following transformation:

$$\psi(x) \xrightarrow{\mathrm{CP}} X_{\mathbf{r}} \overline{\psi}(x_P),$$
(2.2)

with a bar denoting the Hermitian conjugate superfield, and where $x = (t, \mathbf{x}), x_P = (t, -\mathbf{x})$ and $X_{\mathbf{r}}$ is a unitary matrix acting on flavour space [37]. The transformation in eq. (2.2) is commonly referred to as a gCP transformation. In the case of $X_{\mathbf{r}} = \mathbb{1}_{\mathbf{r}}$, one recovers the canonical CP transformation. The action of the gCP transformation on a chiral superfield and, in particular, on its fermionic component is described in detail in appendix A.

The form of the matrix $X_{\mathbf{r}}$ is constrained due to the presence of a flavour symmetry [6, 7]. Performing first a gCP transformation, followed by a flavour symmetry transformation $g \in G_f$, and subsequently an inverse gCP transformation, one finds

$$\psi(x) \xrightarrow{\mathrm{CP}} X_{\mathbf{r}} \overline{\psi}(x_P) \xrightarrow{g} X_{\mathbf{r}} \rho_{\mathbf{r}}^*(g) \overline{\psi}(x_P) \xrightarrow{\mathrm{CP}^{-1}} X_{\mathbf{r}} \rho_{\mathbf{r}}^*(g) X_{\mathbf{r}}^{-1} \psi(x) .$$
(2.3)

 $^{^{1}}$ In what follows we will focus on a supersymmetric construction with global supersymmetry (see subsection 2.2).

The theory should remain invariant under this sequence of transformations, and thus, the resulting transformation must correspond to a flavour symmetry transformation (cf. eq. (2.1)) $\rho_{\mathbf{r}}(g')$, with g' being some element of G_f , i.e., we have:

$$X_{\mathbf{r}} \rho_{\mathbf{r}}^*(g) X_{\mathbf{r}}^{-1} = \rho_{\mathbf{r}}(g'), \quad g, g' \in G_f.$$

$$(2.4)$$

This equation defines the consistency condition, which has to be respected for consistent implementation of a gCP symmetry along with a flavour symmetry, provided the full flavour symmetry group G_f has been correctly identified [6, 7]. Notice that $X_{\mathbf{r}}$ is a unitary matrix defined for each irrep [38]. Several well-known facts about this consistency condition are in order.

- Equation (2.4) has to be satisfied for all irreps \mathbf{r} simultaneously, i.e., the elements g and g' must be the same for all \mathbf{r} .
- For a given irrep **r**, the consistency condition defines $X_{\mathbf{r}}$ up to an overall phase and a G_f transformation.
- It follows from eq. (2.4) that the elements g and g' must be of the same order.
- It is sufficient to impose eq. (2.4) on the generators of a discrete group G_f .
- The chain CP → g → CP⁻¹ maps the group element g onto g' and preserves the flavour symmetry group structure. Therefore, it realises a homomorphism v(g) = g' of G_f. Assuming the presence of faithful representations **r**, i.e., those for which ρ_{**r**} maps each element of G_f to a distinct matrix, eq. (2.4) defines a unique mapping of G_f to itself. In this case, v(g) is an automorphism of G_f.
- The automorphism v(g) = g' must be class-inverting with respect to G_f , i.e. g' and g^{-1} belong to the same conjugacy class [38]. It is furthermore an outer automorphism, meaning no $h \in G_f$ exists such that $g' = h^{-1}gh$.

It has been shown in ref. [6] that under the assumption of $X_{\mathbf{r}}$ being a symmetric matrix,² the full symmetry group is isomorphic to a semi-direct product $G_f \rtimes H_{\mathrm{CP}}$, where $H_{\mathrm{CP}} \simeq \mathbb{Z}_2^{\mathrm{CP}}$ is the group generated by the gCP transformation.

Finally, we would like to note that for $G_f = S_3$, A_4 , S_4 and A_5 and in the bases for their representation matrices summarised in appendix B.2, the gCP transformation $X_{\mathbf{r}} = \mathbb{1}_{\mathbf{r}}$ up to inner automorphisms, i.e, $X_{\mathbf{r}} = \rho_{\mathbf{r}}(g)$, $g \in G_f$, as shown in refs. [7, 8] and [16].

2.2 Modular symmetry and modular-invariant theories

In this subsection, we briefly summarise the modular invariance approach to flavour [21]. An element γ of the modular group $\overline{\Gamma}$ acts on a complex variable τ belonging to the upper-half complex plane as follows:

$$\gamma \tau = \frac{a\tau + b}{c\tau + d}$$
, where $a, b, c, d \in \mathbb{Z}$ and $ad - bc = 1$, $\operatorname{Im} \tau > 0$. (2.5)

²In this case, the CP transformation applied twice to a chiral superfield gives the field itself (see eq. (2.2)). We note also that the CP transformation applied twice to a fermion field gives the field multiplied by a minus sign, which is consistent with the superfield transformation (see appendix A).

The modular group $\overline{\Gamma}$ is isomorphic to the projective special linear group $PSL(2,\mathbb{Z}) = SL(2,\mathbb{Z})/\mathbb{Z}_2$, where $SL(2,\mathbb{Z})$ is the special linear group of integer 2×2 matrices with unit determinant and $\mathbb{Z}_2 = \{I, -I\}$ is its centre, I being the identity element. The group $\overline{\Gamma}$ can be presented in terms of two generators S and T satisfying

$$S^2 = (ST)^3 = I. (2.6)$$

The generators admit the following matrix representation:

$$S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \qquad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}.$$
(2.7)

The action of S and T on τ amounts to inversion with a change of sign and translation, respectively:

$$\tau \xrightarrow{S} -\frac{1}{\tau}, \qquad \tau \xrightarrow{T} \tau + 1.$$
 (2.8)

Let us consider the infinite normal subgroups $\Gamma(N)$, N = 1, 2, 3, ..., of $SL(2, \mathbb{Z})$ (called also the principal congruence subgroups):

$$\Gamma(N) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \operatorname{SL}(2, \mathbb{Z}), \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \pmod{N} \right\}.$$
(2.9)

For N = 1 and 2, one defines the groups $\overline{\Gamma}(N) \equiv \Gamma(N)/\{I, -I\}$ (note that $\overline{\Gamma}(1) \equiv \overline{\Gamma}$), while for N > 2, $\overline{\Gamma}(N) \equiv \Gamma(N)$. The quotient groups $\Gamma_N \equiv \overline{\Gamma}/\overline{\Gamma}(N)$ turn out to be finite. They are referred to as finite modular groups. Remarkably, for $N \leq 5$, these groups are isomorphic to permutation groups: $\Gamma_2 \simeq S_3$, $\Gamma_3 \simeq A_4$, $\Gamma_4 \simeq S_4$ and $\Gamma_5 \simeq A_5$. Their group theory is summarised in appendix B. We recall here only that the group Γ_N is presented by two generators S and T satisfying:

$$S^{2} = (ST)^{3} = T^{N} = I. (2.10)$$

We will work in the basis in which the generators S and T of these groups are represented by symmetric matrices,

$$\rho_{\mathbf{r}}(S) = \rho_{\mathbf{r}}^T(S), \quad \rho_{\mathbf{r}}(T) = \rho_{\mathbf{r}}^T(T), \qquad (2.11)$$

for all irreducible representations **r**. The convenience of this choice will become clear later on. For the groups Γ_N with $N \leq 5$, the working bases are provided in appendix B.2.

The key elements of the considered framework are modular forms $f(\tau)$ of weight k and level N. These are holomorphic functions, which transform under $\overline{\Gamma}(N)$ as follows:

$$f(\gamma\tau) = (c\tau + d)^k f(\tau), \quad \gamma \in \overline{\Gamma}(N), \quad (2.12)$$

where the weight k is an even and non-negative number, and the level N is a natural number. For certain k and N, the modular forms span a linear space of finite dimension. One can find a basis in this space such that a multiplet of modular forms $F(\tau) \equiv (f_1(\tau), f_2(\tau), \dots)^T$ transforms according to a unitary representation **r** of Γ_N :

$$F(\gamma\tau) = (c\tau + d)^k \rho_{\mathbf{r}}(\gamma) F(\tau), \quad \gamma \in \overline{\Gamma}.$$
(2.13)

In appendix C.1, we provide the multiplets of modular forms of lowest non-trivial weight k = 2 at levels N = 2, 3, 4 and 5, i.e., for S_3 , A_4 , S_4 and A_5 . Multiplets of higher weight modular forms can be constructed from tensor products of the lowest weight multiplets. For N = 4 (i.e., S_4), we present in appendix C.3 modular multiplets of weight $k \leq 10$ derived in the symmetric basis for the S_4 generators (see appendix B.2). For N = 3 and N = 5 (i.e., A_4 and A_5), modular multiplets of weight up to 6 and 10, computed in the bases employed by us, can be found in [21] and [32], respectively.

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

$$\mathcal{S} = \int \mathrm{d}^4 x \, \mathrm{d}^2 \theta \, \mathrm{d}^2 \overline{\theta} \, K(\tau, \overline{\tau}, \psi, \overline{\psi}) + \int \mathrm{d}^4 x \, \mathrm{d}^2 \theta \, W(\tau, \psi) + \int \mathrm{d}^4 x \, \mathrm{d}^2 \overline{\theta} \, \overline{W}(\overline{\tau}, \overline{\psi}) \,, \qquad (2.14)$$

where K is the Kähler potential, W is the superpotential, ψ denotes a set of chiral supermultiplets ψ_i , and τ is the modulus chiral superfield, whose lowest component is the complex scalar field acquiring a VEV.³ θ and $\overline{\theta}$ are Graßmann variables. The modulus τ and supermultiplets ψ_i transform under the action of the modular group in a certain way [39, 40]. Assuming, in addition, that the supermultiplets $\psi_i = \psi_i(x)$ transform in a certain irreducible representation \mathbf{r}_i of Γ_N , the transformations read:

$$\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \overline{\Gamma} : \quad \begin{cases} \tau \to \frac{a\tau + b}{c\tau + d}, \\ \psi_i \to (c\tau + d)^{-k_i} \rho_{\mathbf{r}_i}(\gamma) \psi_i. \end{cases}$$
(2.15)

It is worth noting that ψ_i is not a multiplet of modular forms, and hence, the weight $(-k_i)$ can be positive or negative, and can be even or odd. Invariance of the matter action under these transformations implies

$$\begin{cases} W(\tau,\psi) \to W(\tau,\psi), \\ K(\tau,\overline{\tau},\psi,\overline{\psi}) \to K(\tau,\overline{\tau},\psi,\overline{\psi}) + f_K(\tau,\psi) + \overline{f_K}(\overline{\tau},\overline{\psi}), \end{cases}$$
(2.16)

where the second line represents a Kähler transformation.

An example of the Kähler potential, which we will use in what follows, reads:

$$K(\tau,\overline{\tau},\psi,\overline{\psi}) = -\Lambda_0^2 \log(-i\tau + i\overline{\tau}) + \sum_i \frac{|\psi_i|^2}{(-i\tau + i\overline{\tau})^{k_i}}, \qquad (2.17)$$

with Λ_0 having mass dimension one. The superpotential can be expanded in powers of ψ_i as follows:

$$W(\tau,\psi) = \sum_{n} \sum_{\{i_1,\dots,i_n\}} \sum_{s} g_{i_1\dots\,i_n,s} \left(Y_{i_1\dots\,i_n,s}(\tau) \,\psi_{i_1}\dots\psi_{i_n} \right)_{\mathbf{1},s} \,, \tag{2.18}$$

³We will use the same notation τ for the lowest complex scalar component of the modulus superfield and will call this component also "modulus" since in what follows we will be principally concerned with this scalar field.

where 1 stands for an invariant singlet of Γ_N . For each set of n fields $\{\psi_{i_1}, \ldots, \psi_{i_n}\}$, the index s labels the independent singlets. Each of these is accompanied by a coupling constant $g_{i_1 \ldots i_{n,s}}$ and is obtained using a modular multiplet $Y_{i_1 \ldots i_{n,s}}$ of the requisite weight. Indeed, to ensure invariance of W under the transformations in eq. (2.15), the set $Y_{i_1 \ldots i_{n,s}}(\tau)$ of functions must transform in the following way (we omit indices for brevity):

$$Y(\tau) \xrightarrow{\gamma} (c\tau + d)^{k_Y} \rho_{\mathbf{r}_Y}(\gamma) Y(\tau) , \qquad (2.19)$$

where \mathbf{r}_Y is a representation of Γ_N , and k_Y and \mathbf{r}_Y are such that

$$k_Y = k_{i_1} + \dots + k_{i_n} \,, \tag{2.20}$$

$$\mathbf{r}_Y \otimes \mathbf{r}_{i_1} \otimes \ldots \otimes \mathbf{r}_{i_n} \supset \mathbf{1} \,. \tag{2.21}$$

Thus, $Y_{i_1 \dots i_n, s}(\tau)$ represents a multiplet of weight k_Y and level N modular forms transforming in the representation \mathbf{r}_Y of Γ_N (cf. eq. (2.13)).

3 gCP transformations consistent with modular symmetry

As we saw in subsection 2.1, CP transformations can in general be combined with flavour symmetries in a non-trivial way. In the set-up of subsection 2.2, the role of flavour symmetry is played by modular symmetry. In this section, we derive the most general form of a CP transformation consistent with modular symmetry. Unlike the case of discrete flavour symmetries, field transformation properties under CP are restricted to a unique possibility, given the transformation of the modulus (see subsection 3.1) and eq. (2.2). The derivation we are going to present is agnostic to the UV completion of the theory and, in particular, the origin of modular symmetry.

3.1 CP transformation of the modulus au

Let us first apply the consistency condition chain⁴

$$CP \to \gamma \to CP^{-1} = \gamma' \in \overline{\Gamma}$$
 (3.1)

to an arbitrary chiral superfield $\psi(x)$ assigned to an irreducible unitary representation **r** of Γ_N , which transforms as $\psi(x) \to X_{\mathbf{r}} \overline{\psi}(x_P)$ under CP:

$$\psi(x) \xrightarrow{\mathrm{CP}} X_{\mathbf{r}} \overline{\psi}(x_P) \xrightarrow{\gamma} (c\tau^* + d)^{-k} X_{\mathbf{r}} \rho_{\mathbf{r}}^*(\gamma) \overline{\psi}(x_P)$$
$$\xrightarrow{\mathrm{CP}^{-1}} (c\tau_{\mathrm{CP}^{-1}}^* + d)^{-k} X_{\mathbf{r}} \rho_{\mathbf{r}}^*(\gamma) X_{\mathbf{r}}^{-1} \psi(x) , \qquad (3.2)$$

where $\tau_{\rm CP^{-1}}$ is the result of applying CP^{-1} to the modulus τ . The resulting transformation should be equivalent to a modular transformation γ' which depends on γ and maps $\psi(x)$ to $(c'\tau + d')^{-k}\rho_{\bf r}(\gamma')\psi(x)$. Taking this into account, we get

$$X_{\mathbf{r}} \rho_{\mathbf{r}}^*(\gamma) X_{\mathbf{r}}^{-1} = \left(\frac{c'\tau + d'}{c\tau_{\mathrm{CP}^{-1}}^* + d}\right)^{-k} \rho_{\mathbf{r}}(\gamma') \,. \tag{3.3}$$

 $^{{}^{4}}$ It may be possible to generalise the CP transformation such that it can be combined not only with modular but also with other internal symmetries of the theory. We are not going to consider this case here.

Since the matrices $X_{\mathbf{r}}$, $\rho_{\mathbf{r}}(\gamma)$ and $\rho_{\mathbf{r}}(\gamma')$ are independent of τ , the overall coefficient on the right-hand side has to be a constant:⁵

$$\frac{c'\tau + d'}{c\tau_{\rm CP^{-1}}^* + d} = \frac{1}{\lambda^*},\tag{3.4}$$

where $\lambda \in \mathbb{C}$, and $|\lambda| = 1$ due to unitarity of $\rho_{\mathbf{r}}(\gamma)$ and $\rho_{\mathbf{r}}(\gamma')$. The values of λ , c' and d' depend on γ .

Taking $\gamma = S$, so that c = 1, d = 0, and denoting c'(S) = C, d'(S) = D while keeping henceforth the notation $\lambda(S) = \lambda$, we find $\tau = (\lambda \tau_{CP^{-1}}^* - D)/C$, and consequently,

$$\tau \xrightarrow{\mathrm{CP}^{-1}} \tau_{\mathrm{CP}^{-1}} = \lambda \left(C\tau^* + D \right), \quad \tau \xrightarrow{\mathrm{CP}} \tau_{\mathrm{CP}} = \frac{1}{C} \left(\lambda \tau^* - D \right).$$
 (3.5)

Let us now act with the chain $CP \to T \to CP^{-1}$ on the modulus τ itself:

$$\tau \xrightarrow{\mathrm{CP}} \frac{1}{C} (\lambda \tau^* - D) \xrightarrow{T} \frac{1}{C} (\lambda (\tau^* + 1) - D) \xrightarrow{\mathrm{CP}^{-1}} \tau + \frac{\lambda}{C}.$$
 (3.6)

The resulting transformation has to be a modular transformation, therefore $\lambda/C \in \mathbb{Z}$. Since $|\lambda| = 1$, we immediately find |C| = 1, $\lambda = \pm 1$. After choosing the sign of C as $C = \mp 1$ so that Im $\tau_{\rm CP} > 0$, the CP transformation rule (3.5) simplifies to

$$\tau \xrightarrow{\text{CP}} n - \tau^*,$$
 (3.7)

with $n \in \mathbb{Z}$. One can easily check that the chain $CP \to S \to CP^{-1} = \gamma'(S)$ (applied to the modulus τ itself) imposes no further restrictions on the form of τ_{CP} . Since S and T generate the entire modular group, we conclude that eq. (3.7) is the most general CP transformation of the modulus τ compatible with the modular symmetry.

It is always possible to redefine the CP transformation in such a way that n = 0. Consider the composition $CP' \equiv T^{-n} \circ CP$ so that $\tau \xrightarrow{CP'} -\tau^*$. It is worth noting that this redefinition represents an inner automorphism which does not spoil the form of gCP transformation in eq. (2.2). Indeed, the chiral superfields transform under CP' as

$$\psi \xrightarrow{\operatorname{CP}'} \rho_{\mathbf{r}}^{-n}(T) X_{\mathbf{r}} \overline{\psi}.$$
(3.8)

Thus, CP' has the same properties as the original CP transformation up to a redefinition of $X_{\mathbf{r}}$. Therefore, from now on we will assume without loss of generality that the modulus τ transforms under CP as⁶

$$\tau \xrightarrow{\text{CP}} -\tau^*. \tag{3.9}$$

It obviously follows from the preceding equation that τ does not change under the action of CP^2 :

$$\tau \xrightarrow{\text{CP}^2} \tau$$
. (3.10)

Thus, in what concerns the action on the modulus τ we have: $CP^2 = I$, $CP^{-1} = CP$.

⁵Strictly speaking, this is only true for non-zero weights k. We assume that at least one superfield with non-zero modular weight exists in the theory, because otherwise the modulus has no effect on the superfield transformations, and the modular symmetry approach reduces to the well-known discrete symmetry approach to flavour.

⁶The CP transformation of the modulus derived by us from the requirement of consistency between modular and CP symmetries has appeared in the context of string-inspired models (see, e.g., refs. [36, 41–43]).

3.2 Extended modular group

Having derived the explicit form of the CP transformation for the modulus τ , we are now in a position to find the action of CP on the modular group $\overline{\Gamma}$ as an outer automorphism $u(\gamma)$. For any modular transformation $\gamma \in \overline{\Gamma}$ we have

$$\tau \xrightarrow{\text{CP}} -\tau^* \xrightarrow{\gamma} -\frac{a\tau^*+b}{c\tau^*+d} \xrightarrow{\text{CP}^{-1}} \frac{a\tau-b}{-c\tau+d}.$$
(3.11)

This implies that the sought-after automorphism is

$$\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \to u(\gamma) \equiv \operatorname{CP} \gamma \operatorname{CP}^{-1} = \begin{pmatrix} a & -b \\ -c & d \end{pmatrix}.$$
(3.12)

In particular, one has (CP) $S(CP)^{-1} = S$, (CP) $T(CP)^{-1} = T^{-1}$, or simply u(S) = S and $u(T) = T^{-1}$. It is straightforward to check that the mapping (3.12) is indeed an outer automorphism of $\overline{\Gamma}$.⁷ Notice further that if $\gamma \in \overline{\Gamma}(N)$, then also $u(\gamma) \in \overline{\Gamma}(N)$.

By adding the CP transformation (3.9) as a new generator to the modular group, one obtains the so-called *extended modular group*:

$$\overline{\Gamma}^* = \left\langle \tau \xrightarrow{T} \tau + 1, \tau \xrightarrow{S} -1/\tau, \tau \xrightarrow{\text{CP}} -\tau^* \right\rangle$$
(3.13)

(see, e.g., [44]), which has a structure of a semi-direct product $\overline{\Gamma}^* \simeq \overline{\Gamma} \rtimes \mathbb{Z}_2^{CP}$, with $\mathbb{Z}_2^{CP} = \{I, \tau \to -\tau^*\}$. The group $\overline{\Gamma}^*$ is isomorphic to the group $\mathrm{PGL}(2,\mathbb{Z})$ of integral 2×2 matrices with determinant ± 1 , the matrices M and -M being identified. The CP transformation is then represented by the matrix

$$CP = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad CP \gamma CP^{-1} = u(\gamma).$$
(3.14)

The action of $\overline{\Gamma}^*$ on the complex upper-half plane is defined as

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \overline{\Gamma}^* : \begin{cases} \tau \to \frac{a\tau + b}{c\tau + d} & \text{if } ad - bc = 1, \\ \tau \to \frac{a\tau^* + b}{c\tau^* + d} & \text{if } ad - bc = -1. \end{cases}$$
(3.15)

3.3 CP transformation of chiral superfields

A chiral superfield $\psi(x)$ transforms according to eq. (2.2) under CP. The consistency condition chain (3.1) applied to ψ constrains the form of its CP transformation matrix $X_{\mathbf{r}}$ as in eq. (3.3), with the overall coefficient on the right-hand side being constant, as discussed earlier, see eq. (3.4). Since $\lambda = \pm 1$, the coefficient on the right-hand side of eq. (3.3) is $(\pm 1)^k$. This sign is actually determined by the signs of matrices in the outer automorphism (3.12), which are unphysical in a modular symmetric theory. By choosing⁸ these

⁷One can explicitly check that i) $u(\gamma_1)u(\gamma_2) = u(\gamma_1\gamma_2)$, meaning u is an automorphism, and that ii) there is no group element $\tilde{\gamma} \in \overline{\Gamma}$ such that $u(\gamma) = \tilde{\gamma}^{-1}\gamma \tilde{\gamma}$, meaning that u is an outer automorphism.

⁸This choice is possible since in the presence of fields with an odd modular weight the theory automatically respects a sign-flip \mathbb{Z}_2 symmetry, which acts only non-trivially on these fields. This implies that the discussed sign is unphysical.

signs in such a way that c' = -c, d' = d, in accordance with eq. (3.12), we obtain a trivial coefficient +1, and the constraint on $X_{\mathbf{r}}$ reduces to

$$X_{\mathbf{r}} \rho_{\mathbf{r}}^*(\gamma) X_{\mathbf{r}}^{-1} = \rho_{\mathbf{r}}(\gamma') \,. \tag{3.16}$$

The constraint we get coincides with the corresponding constraint in the case of non-Abelian discrete flavour symmetries, eq. (2.4). However, unlike in the usual discrete flavour symmetry approach, modular symmetry restricts the form of the automorphism $\gamma \to \gamma' = u(\gamma)$ to the unique possibility given in eq. (3.12), which acts on the generators as $S \to u(S) = S$ and $T \to u(T) = T^{-1}$. Therefore, for each irreducible representation \mathbf{r} , $X_{\mathbf{r}}$ in eq. (3.16) is fixed up to an overall phase by Schur's lemma.

For the working bases discussed in subsection 2.2 and given in appendix B.2, one has $X_{\mathbf{r}} = \mathbb{1}_{\mathbf{r}}$, i.e., the gCP transformation has the canonical form. The key feature of the aforementioned bases which allows for this simplification is that the group generators S and T are represented by symmetric matrices. Indeed, if eq. (2.11) holds, one has:

$$\rho_{\mathbf{r}}^{*}(S) = \rho_{\mathbf{r}}^{\dagger}(S) = \rho_{\mathbf{r}}(S^{-1}) = \rho_{\mathbf{r}}(S), \quad \rho_{\mathbf{r}}^{*}(T) = \rho_{\mathbf{r}}^{\dagger}(T) = \rho_{\mathbf{r}}(T^{-1}), \quad (3.17)$$

so that $X_{\mathbf{r}} = \mathbb{1}_{\mathbf{r}}$ solves the consistency condition (3.16).

3.4 CP transformation of modular form multiplets

Since modular multiplets $Y(\tau)$ transform under the modular group in essentially the same way as chiral superfields, it is natural to expect that the above discussion holds for modular multiplets as well. In particular, they should transform under CP as $Y \to X_r Y^*$. Still, it is instructive to derive their transformation rule explicitly.

Under a modular transformation, $Y(\tau)$ transforms as in eq. (2.19), while under the action of CP one has $Y(\tau) \to Y(-\tau^*)$. It can be shown (see appendix D of [31]) that the complex-conjugated CP-transformed multiplets $Y^*(-\tau^*)$ transform almost like the original multiplets $Y(\tau)$ under a modular transformation, namely:

$$Y^{*}(-\tau^{*}) \xrightarrow{\gamma} Y^{*}(-(\gamma\tau)^{*}) = Y^{*}(u(\gamma)(-\tau^{*})) = (c\tau+d)^{k} \rho_{\mathbf{r}}^{*}(u(\gamma)) Y^{*}(-\tau^{*}), \quad (3.18)$$

for a multiplet $Y(\tau)$ of weight k transforming in the irreducible representation **r** of Γ_N .

Using the consistency condition in eq. (3.16), one then sees that it is the object $X_{\mathbf{r}}^T Y^*(-\tau^*)$ which transforms like $Y(\tau)$ under a modular transformation, i.e.:

$$X_{\mathbf{r}}^T Y^*(-\tau^*) \xrightarrow{\gamma} (c\tau+d)^k \rho_{\mathbf{r}}(\gamma) \left[X_{\mathbf{r}}^T Y^*(-\tau^*) \right].$$
(3.19)

If there exists a unique modular form multiplet at a certain level N, weight k and representation \mathbf{r} , then proportionality follows:

$$Y(\tau) = z X_{\mathbf{r}}^T Y^*(-\tau^*), \qquad (3.20)$$

with $z \in \mathbb{C}$. This is indeed the case for $2 \leq N \leq 5$ and lowest weight k = 2. Since $Y(-(-\tau^*)^*) = Y(\tau)$, it follows that $X_{\mathbf{r}} X_{\mathbf{r}}^* = |z|^2 \mathbb{1}_{\mathbf{r}}$, implying i) that $z = e^{i\phi}$ is a phase

which can be absorbed in the normalisation of $Y(\tau)$, and ii) that $X_{\mathbf{r}}$ must be symmetric in this case, $X_{\mathbf{r}} X_{\mathbf{r}}^* = \mathbb{1}_{\mathbf{r}} \Rightarrow X_{\mathbf{r}} = X_{\mathbf{r}}^T$, independently of the basis. One can then write

$$Y(\tau) \xrightarrow{\text{CP}} Y(-\tau^*) = X_{\mathbf{r}} Y^*(\tau)$$
(3.21)

for these multiplets, as anticipated.

As we have seen in subsection 3.3, in a basis in which the generators S and T of Γ_N are represented by symmetric matrices, one has $X_{\mathbf{r}} = \mathbb{1}_{\mathbf{r}}$. From eq. (3.20) it follows that $Y(-\tau^*) = e^{i\phi} Y^*(\tau)$, the phase ϕ being removable, as commented above. At the q-expansion level this means that, in such a basis, all the expansion coefficients are real up to a common complex phase. This is indeed the case for the lowest-weight modular form multiplets of Γ_N with $N \leq 5$, as can be explicitly verified from the q-expansions collected in appendix C.2. This is further the case for the higher-weight modular multiplets of these groups in such a basis, given the reality of Clebsch-Gordan coefficients, summarised in appendix B.3.

4 CP-invariant theories with modular symmetry

4.1 Implications of CP invariance for the couplings

We have found so far that a CP transformation consistent with modular symmetry acts on fields and modular form multiplets in the following way:

$$\tau \xrightarrow{\text{CP}} -\tau^*, \quad \psi(x) \xrightarrow{\text{CP}} X_{\mathbf{r}} \overline{\psi}(x_P), \quad Y(\tau) \xrightarrow{\text{CP}} Y(-\tau^*) = X_{\mathbf{r}} Y^*(\tau).$$
(4.1)

A SUSY modular-invariant theory is thus CP-conserving if the transformation (4.1) leaves the matter action S given by eq. (2.14) unchanged. In particular, the superpotential Whas to transform into its Hermitian conjugate, while the Kähler potential K is allowed to change by a Kähler transformation.

The Kähler potential of eq. (2.17) is clearly invariant under the CP transformation (4.1), since it depends on $|\psi|^2$ and Im τ , both of which remain unchanged (up to a change $x \to x_P$ which does not affect S). On the other hand, the superpotential can be written as a sum of independent terms of the form

$$W \supset \sum_{s} g_s \left(Y_s(\tau) \psi_1 \dots \psi_n \right)_{\mathbf{1},s} , \qquad (4.2)$$

where $Y_s(\tau)$ are modular multiplets of a certain weight and irreducible representation, and g_s are complex coupling constants, see eq. (2.18). Such terms transform non-trivially under CP, which leads to a certain constraint on the couplings g_s .

This can be easily checked for a symmetric basis, as in this basis $X_{\mathbf{r}} = \mathbb{1}_{\mathbf{r}}$ for any representation \mathbf{r} , so that one has (assuming proper normalisation of the modular multiplets $Y_s(\tau)$)

$$g_{s}(Y_{s}(\tau)\psi_{1}\dots\psi_{n})_{\mathbf{1},s} \xrightarrow{\mathrm{CP}} g_{s}\left(Y_{s}(-\tau^{*})\overline{\psi}_{1}\dots\overline{\psi}_{n}\right)_{\mathbf{1},s} = g_{s}\left(Y_{s}^{*}(\tau)\overline{\psi}_{1}\dots\overline{\psi}_{n}\right)_{\mathbf{1},s} = g_{s}\overline{(Y_{s}(\tau)\psi_{1}\dots\psi_{n})_{\mathbf{1},s}},$$

$$(4.3)$$

where in the last equality we have used the reality of the Clebsch-Gordan coefficients, which holds for $N \leq 5$. It is now clear that a term in the sum of eq. (4.2) transforms into the Hermitian conjugate of

$$g_s^* \left(Y_s(\tau) \psi_1 \dots \psi_n \right)_{\mathbf{1},s} , \qquad (4.4)$$

which should coincide with the original term due to the independence of singlets in eq. (4.2). It now follows that $g_s = g_s^*$, i.e., all coupling constants g_s have to be real to conserve CP.

As a final remark, let us denote by \tilde{g}_s the couplings written for a general basis and arbitrary normalisation of the modular form multiplets. The CP constraint on \tilde{g}_s is then more complicated, since the singlets of different bases coincide only up to normalisation factors, determined by the choice of normalisations of the Clebsch-Gordan coefficients and of the modular form multiplets. Since the normalisation factors can differ between singlets, the corresponding couplings \tilde{g}_s may require non-trivial phases to conserve CP. These phases can be found directly by performing a basis transformation and matching \tilde{g}_s to g_s in the symmetric basis (and with proper modular form multiplet normalisation).

4.2 Implications of CP invariance for the mass matrices

As a more concrete example, let us consider the Yukawa coupling term

$$W_L = \sum_{s} g_s \left(Y_s(\tau) E^c L H_d \right)_{1,s} , \qquad (4.5)$$

which gives rise to the charged lepton mass matrix. Here E^c is a modular symmetry multiplet of SU(2) charged lepton singlets, L is a modular symmetry multiplet of SU(2) lepton doublets, and H_d is a Higgs doublet which transforms trivially under modular symmetry and whose neutral component acquires a VEV $v_d = \langle H_d^0 \rangle$ after electroweak symmetry breaking.

Expanding the singlets, one gets

$$W_L = \sum_s g_s \lambda_{ij}^s(\tau) E_i^c L_j H_d \equiv \lambda_{ij}(\tau) E_i^c L_j H_d , \qquad (4.6)$$

where entries of the matrices $\lambda_{ij}^s(\tau)$ are formed from components of the corresponding modular multiplets $Y_s(\tau)$. In a general basis, superfields transform under CP as

$$E^c \xrightarrow{\mathrm{CP}} X_R^* \overline{E^c}, \quad L \xrightarrow{\mathrm{CP}} X_L \overline{L}, \quad H_d \xrightarrow{\mathrm{CP}} \eta_d \overline{H_d},$$

$$(4.7)$$

and we set $\eta_d = 1$ without loss of generality. It follows that

$$W_L \xrightarrow{\text{CP}} \left(X_R^{\dagger} \lambda(-\tau^*) X_L \right)_{ij} \overline{E_i^c} \overline{L_j} \overline{H_d} , \qquad (4.8)$$

so that CP conservation implies

$$X_R^{\dagger} \lambda(-\tau^*) X_L = \lambda^*(\tau) .$$
(4.9)

The resulting charged lepton mass matrix $M_e = v_d \lambda^{\dagger}$ (written in the left-right convention) satisfies

$$X_L^{\dagger} M_e(-\tau^*) X_R = M_e^*(\tau) , \qquad (4.10)$$

which coincides with the corresponding constraint in the case of CP invariance combined with discrete flavour symmetry, apart from the fact that now the mass matrix depends on the modulus τ which also transforms under CP. Similarly, for the neutrino Majorana mass matrix M_{ν} one has

$$X_L^T M_\nu(-\tau^*) X_L = M_\nu^*(\tau) \,. \tag{4.11}$$

Note that matrix X_L is the same in eqs. (4.10) and (4.11) since left-handed charged leptons l_L and left-handed neutrinos ν_{lL} form an electroweak SU(2) doublet L, so they transform uniformly both under CP and modular transformations:

$$X_{l_{L}} = X_{\nu_{lL}} \equiv X_{L}, \quad \rho_{l_{L}}(\gamma) = \rho_{\nu_{lL}}(\gamma) \equiv \rho_{L}(\gamma), \quad k_{l_{L}} = k_{\nu_{lL}} \equiv k_{L}.$$
(4.12)

This can also be found directly from the form of the charged current (CC) weak interaction Lagrangian

$$\mathcal{L}_{\rm CC} = -\frac{g}{\sqrt{2}} \sum_{l=e,\mu,\tau} \overline{l_L} \, \gamma_\alpha \, \nu_{lL} \, W^{\alpha \dagger} + \text{h.c.}$$
(4.13)

by ensuring its CP invariance.⁹

In a symmetric basis $X_L = X_R = 1$, the constraints on the mass matrices simplify to

$$M_e(-\tau^*) = M_e^*(\tau), \quad M_\nu(-\tau^*) = M_\nu^*(\tau),$$
(4.14)

which further reduce to reality of the couplings. Namely, for the charged lepton mass matrix one has

$$M_e(-\tau^*) = v_d \sum_s g_s^* (\lambda^s)^{\dagger}(-\tau^*) = v_d \sum_s g_s^* (\lambda^s)^T(\tau) ,$$

$$M_e^*(\tau) = \left(v_d \sum_s g_s^* (\lambda^s)^{\dagger}(\tau) \right)^* = v_d \sum_s g_s (\lambda^s)^T(\tau) .$$
(4.15)

Clearly, CP invariance requires $g_s = g_s^*$, since $\lambda^s(\tau)$ are linearly independent matrices, which in turn is guaranteed by independence of the singlets.

4.3 CP-conserving values of the modulus au

In a CP-conserving modular-invariant theory both CP and modular symmetry are broken spontaneously by the VEV of the modulus τ . However, there exist certain values of τ which conserve CP, while breaking the modular symmetry. Obviously, this is the case if τ is left invariant by CP, i.e.

$$\tau \xrightarrow{\text{CP}} -\tau^* = \tau \,, \tag{4.16}$$

meaning that τ lies on the imaginary axis, $\operatorname{Re} \tau = 0$. In a symmetric basis one then has

$$M_e(\tau) = M_e^*(\tau), \quad M_\nu(\tau) = M_\nu^*(\tau),$$
 (4.17)

⁹Since the original superfields in a modular-invariant theory are not normalised canonically, there is actually a prefactor of $(2 \operatorname{Im} \tau)^{-k_L}$ in the CC weak interaction Lagrangian which originates from the Kähler potential. This prefactor is necessary for modular invariance in order to compensate the weights $k_{l_L} = k_{\nu_{lL}} \equiv k_L$.

as can be seen from eq. (4.14). The resulting mass matrices are real and the corresponding CPV phases are trivial, such that $\sin \delta = \sin \alpha_{21} = \sin \alpha_{31} = 0$ in the standard parametrisation [45] of the PMNS mixing matrix.

Let us now consider a point $\gamma \tau$ in the plane of the modulus related to a CP-invariant point $\tau = -\tau^*$ by a modular transformation γ . This point is physically equivalent to τ due to modular invariance and therefore it should also be CP-conserving. However, $\gamma \tau$ does not go to itself under CP. Instead, one has

$$\gamma \tau \xrightarrow{\text{CP}} (\gamma \tau)_{\text{CP}} = u(\gamma) \tau_{\text{CP}} = u(\gamma) \tau = u(\gamma) \gamma^{-1} \gamma \tau,$$
 (4.18)

so the resulting CP-transformed value $(\gamma \tau)_{\rm CP}$ is related to the original value $\gamma \tau$ by a modular transformation $u(\gamma)\gamma^{-1}$.

Hence, it is natural to expect that a value of τ conserves CP if it is left invariant by CP up to a modular transformation, i.e.,

$$\tau \xrightarrow{\text{CP}} -\tau^* = \gamma \tau \tag{4.19}$$

for some $\gamma \in \overline{\Gamma}$.¹⁰ Indeed, one can check that modular invariance of the mass terms requires the mass matrices to transform under a modular transformation as

$$M_e(\tau) \xrightarrow{\gamma} M_e(\gamma\tau) = \rho_L(\gamma) M_e(\tau) \rho_E^T(\gamma),$$

$$M_\nu(\tau) \xrightarrow{\gamma} M_\nu(\gamma\tau) = \rho_L^*(\gamma) M_\nu(\tau) \rho_L^{\dagger}(\gamma),$$
(4.20)

where ρ_L and ρ_E are the representation matrices for the SU(2) lepton doublet L and charged lepton singlets E^c , respectively. We have also taken into account the rescaling of fields due to the non-canonical form of the Kähler potential (2.17), which leads to cancellation of the modular weights in the transformed mass matrices.

It is clear from eq. (4.20) that mass eigenvalues are unaffected by the replacement $\tau \to \gamma \tau$ in the mass matrices. Moreover, the unitary rotations U_e and U_{ν} diagonalising the mass matrices $M_e M_e^{\dagger}$ and M_{ν} respectively transform as

$$U_e \xrightarrow{\gamma} \rho_L U_e, \quad U_\nu \xrightarrow{\gamma} \rho_L U_\nu, \qquad (4.21)$$

so the PMNS mixing matrix $U_{\text{PMNS}} = U_e^{\dagger} U_{\nu}$ does not change. This means that the mass matrices evaluated at points τ and $\gamma \tau$ lead to the same values of physical observables.

If we now consider a value of τ which satisfies eq. (4.19), then in a symmetric basis we have

$$M_e(\gamma \tau) = M_e^*(\tau), \quad M_\nu(\gamma \tau) = M_\nu^*(\tau),$$
 (4.22)

from eq. (4.14). It follows from the above discussion that the observables evaluated at τ coincide with their complex conjugates, hence CPV phases are trivial (0 or π).

To find all points satisfying eq. (4.19), it is sufficient to restrict ourselves to the fundamental domain \mathcal{D} of the modular group given by

$$\mathcal{D} = \left\{ \tau \in \mathbb{C} : \quad \operatorname{Im} \tau > 0 \,, \quad |\operatorname{Re} \tau| \le \frac{1}{2} \,, \quad |\tau| \ge 1 \right\}, \tag{4.23}$$

¹⁰A similar condition has been derived in ref. [42] in the context of string theories (in which the CP symmetry represents a discrete gauge symmetry), postulating the action of CP on the compactified directions.

since all other points are physically equivalent to the points from \mathcal{D} . All CP-conserving values of τ outside the fundamental domain are related to the CP-conserving values of τ within the fundamental domain by modular transformations.

The interior of \mathcal{D} , which we denote as $\operatorname{int}(\mathcal{D})$, maps to itself under CP. Apart from that, no two points from $\operatorname{int}(\mathcal{D})$ are related by any non-trivial modular transformation. Therefore, if $\tau \in \operatorname{int}(\mathcal{D})$, then eq. (4.19) reduces to eq. (4.16) and we find again $\operatorname{Re} \tau = 0$. The remaining possibility is that τ lies on the boundary of \mathcal{D} . Then it is easy to show that it also satisfies eq. (4.19), but with a non-trivial γ . Namely, for the left vertical line we have $\tau = -1/2 + i y \xrightarrow{\operatorname{CP}} 1/2 + i y = T\tau$, while for the arc we have $\tau = e^{i\varphi} \xrightarrow{\operatorname{CP}} -e^{-i\varphi} = S\tau$.

We conclude that CP-conserving values of τ are the imaginary axis and the boundary of the fundamental domain \mathcal{D} . These values can also be obtained by algebraically solving eq. (4.19), by noticing that it implies $u(\gamma)\gamma = I$ and using the requirement that $\gamma\tau$ belongs to the fundamental domain.

Thus, at the left and right vertical boundaries as well as at the arc boundary of the fundamental domain and at the imaginary axis within it, i.e., at $\tau_{LB} = -1/2 + iy$, $\tau_{RB} = 1/2 + iy$, $y \ge \sqrt{3}/2$, at $\tau_{AB} = e^{i\varphi}$, $\varphi = [60^{\circ}, 120^{\circ}]$, and at $\tau_{IA} = iy$, $y \ge 1$, we have a \mathbb{Z}_2^{CP} symmetry. At the left and right cusps of the fundamental domain, $\tau_L = -1/2 + i\sqrt{3}/2$ and $\tau_R = 1/2 + i\sqrt{3}/2$, and at $\tau_C = i$, the symmetry is enhanced to $\mathbb{Z}_2^{\text{CP}} \times \mathbb{Z}_3^{ST}$, $\mathbb{Z}_2^{\text{CP}} \times \mathbb{Z}_3^{TS}$ and $\mathbb{Z}_2^{\text{CP}} \times \mathbb{Z}_2^{S}$, respectively [31], while at $\tau_T = i\infty$, the symmetry in the case of Γ_N is enhanced to $\mathbb{Z}_2^{\text{CP}} \times \mathbb{Z}_N^T$ [29, 31].

5 Example: CP-invariant modular S_4 models

To illustrate the use of gCP invariance combined with modular symmetry for model building, we consider modular $\Gamma_4 \simeq S_4$ models of lepton masses and mixing, in which neutrino masses are generated via the type I seesaw mechanism. Such models have been extensively studied in ref. [31] in the context of plain modular symmetry without gCP invariance. Here we briefly summarise the construction of ref. [31] and investigate additional constraints on the models imposed by CP invariance, having the modulus τ as the only potential source of CPV.

Representations of the superfields under the modular group are chosen as follows:

- Higgs doublets H_u and H_d (with $\langle H_u^0 \rangle = v_u$) are S_4 trivial singlets of zero weight: $\rho_u = \rho_d \sim \mathbf{1}$ and $k_u = k_d = 0$;
- lepton SU(2) doublets L and neutral lepton gauge singlets N^c form S_4 triplets ($\rho_L \sim \mathbf{3}$ or $\mathbf{3}'$, $\rho_N \sim \mathbf{3}$ or $\mathbf{3}'$) of weights k_L and k_N , respectively;
- charged lepton singlets E_1^c , E_2^c and E_3^c transform as S_4 singlets ($\rho_{1,2,3} \sim \mathbf{1}$ or $\mathbf{1'}$) of weights $k_{1,2,3}$.

The relevant superpotential terms read

$$W = \sum_{i=1}^{3} \alpha_i \left(E_i^c L Y^{(k_{\alpha_i})} \right)_{\mathbf{1}} H_d + g \left(N^c L Y^{(k_g)} \right)_{\mathbf{1}} H_u + \Lambda \left(N^c N^c Y^{(k_\Lambda)} \right)_{\mathbf{1}}, \tag{5.1}$$

where $Y^{(k)}$ denotes a modular multiplet of weight k and level 4, and a sum over all independent singlets with the coefficients $\alpha_i = (\alpha_i, \alpha'_i, \ldots), g = (g, g', \ldots)$ and $\Lambda = (\Lambda, \Lambda', \ldots)$ is implied. It has been found in ref. [31] that the minimal (in terms of the total number of parameters) viable choice of modular weights and representations is

$$k_{\alpha_1} = 2, \qquad k_{\alpha_2} = k_{\alpha_3} = 4, \qquad k_g = 2, \qquad k_{\Lambda} = 0, \rho_L \sim \mathbf{3}, \qquad \rho_1 \sim \mathbf{1}', \qquad \rho_2 \sim \mathbf{1}, \qquad \rho_3 \sim \mathbf{1}', \qquad \rho_N \sim \mathbf{3} \text{ or } \mathbf{3}',$$
(5.2)

which leads to the superpotential of the form

$$W = \alpha \left(E_{1}^{c} L Y_{\mathbf{3'}}^{(2)} \right)_{\mathbf{1}} H_{d} + \beta \left(E_{2}^{c} L Y_{\mathbf{3}}^{(4)} \right)_{\mathbf{1}} H_{d} + \gamma \left(E_{3}^{c} L Y_{\mathbf{3'}}^{(4)} \right)_{\mathbf{1}} H_{d} + g \left(N^{c} L Y_{\mathbf{2}}^{(2)} \right)_{\mathbf{1}} H_{u} + g' \left(N^{c} L Y_{\mathbf{3'}}^{(2)} \right)_{\mathbf{1}} H_{u} + \Lambda \left(N^{c} N^{c} \right)_{\mathbf{1}} ,$$
(5.3)

where the multiplets of modular forms $Y_{2,3'}^{(2)}$ and $Y_{3,3'}^{(4)}$ have been derived in ref. [30]. Here no sums are implied, since each singlet is unique, and the coefficients $(\alpha, \beta, \gamma) = (\alpha_1, \alpha_2, \alpha_3)$, g and Λ are real without loss of generality, as the corresponding phases can be absorbed into the fields E_1^c , E_2^c , E_3^c , L and N^c , respectively. Therefore, the only complex parameter of the theory is g'/g. If a symmetric basis is used and the modular form multiplets are properly normalised, then CP is conserved whenever

$$\operatorname{Im}\left(g'/g\right) = 0. \tag{5.4}$$

The basis used in ref. [31] is not symmetric. One can check that it can be related to the symmetric basis here considered by the following transformation matrices $U_{\mathbf{r}}$:

$$U_{1} = U_{1'} = 1, \qquad U_{2} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix},$$

$$U_{3} = U_{3'} = \frac{1}{2\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -e^{-i\pi/4} & 0 \\ 0 & 0 & -e^{i\pi/4} \end{pmatrix} \begin{pmatrix} 2 & 2 & 2 \\ -2 & 1 + \sqrt{3} & 1 - \sqrt{3} \\ -2 & 1 - \sqrt{3} & 1 + \sqrt{3} \end{pmatrix}.$$
 (5.5)

By direct comparison of the singlets $(N^c L Y_2^{(2)})_1$ and $(N^c L Y_{3'}^{(2)})_1$ written in different bases, and taking into account an extra factor of *i* arising from the normalisation of the modular form multiplets used in ref. [31], we find that also in this basis CP invariance results in the condition (5.4). In what follows, we report the parameter values in the basis of ref. [31] for ease of comparison.

Through numerical search, five viable pairs of regions of the parameter space have been found in ref. [31], denoted as A and A^{*}, B and B^{*}, etc. with the starred regions corresponding to CP-conjugated models $\tau \to -\tau^*$, $(g'/g) \to (g'/g)^*$ predicting the opposite values of the CPV phases. Among these five pairs of regions only one pair (A and A^{*}, for which $\rho_N \sim 3'$) is consistent with the condition (5.4), and only a small portion of the parameter space is allowed. We report the corresponding best fit values and the confidence intervals of the parameters and observables in table 1.

This minimal CP-invariant model, predicting 12 observables, is characterised by 7 parameters: the 6 real parameters $v_d \alpha$, β/α , γ/α , $v_u^2 g^2/\Lambda$, g'/g, Im τ and the phase

| $\mathbf{D} + \mathbf{C} + 1$ | 2 | 2 | |
|-------------------------------|--|---|--|
| | ~ | 3σ range | |
| | · · · · · · · · · · · · · · · · · · · | $\pm (0.09371 - 0.1049)$ | |
| 1.016 | 1.015 - 1.017 | 1.014 - 1.018 | |
| 9.348 | 8.426 - 11.02 | 7.845 - 12.25 | |
| 0.002203 | 0.002046 - 0.00236 | 0.001954 - 0.00246 | |
| -0.02093 | -(0.01846 - 0.02363) | -(0.01682 - 0.02528) | |
| 53.61 | | | |
| 0.0135 | | | |
| 0.004796 | 0.004454 - 0.005135 | 0.004251 - 0.005351 | |
| 0.05756 | 0.0488 - 0.06388 | 0.04399 - 0.06861 | |
| 0.02981 | 0.02856 - 0.0312 | 0.02769 - 0.03212 | |
| 7.326 | 7.109 - 7.551 | 6.953 - 7.694 | |
| 2.457 | 2.421 - 2.489 | 2.396 - 2.511 | |
| 0.305 | 0.2825 - 0.3281 | 0.2687 - 0.3427 | |
| 0.02136 | 0.02012 - 0.02282 | 0.0192 - 0.02372 | |
| 0.4862 | 0.4848 - 0.4873 | 0.484 - 0.4882 | |
| NO | | | |
| 0.01211 | 0.01195 - 0.01226 | 0.01185 - 0.01236 | |
| 0.01483 | 0.01477 - 0.01489 | 0.01473 - 0.01493 | |
| 0.05139 | 0.051 - 0.05172 | 0.05074 - 0.05195 | |
| 0.07833 | 0.07774 - 0.07886 | 0.07734 - 0.07921 | |
| 0.01201 | 0.01187 - 0.01213 | 0.01178 - 0.01221 | |
| ± 1.641 | $\pm (1.633 - 1.651)$ | $\pm (1.627 - 1.656)$ | |
| ± 0.3464 | $\pm (0.3335 - 0.3618)$ | $\pm (0.324 - 0.3713)$ | |
| ± 1.254 | $\pm (1.238 - 1.271)$ | $\pm(1.229 - 1.283)$ | |
| 1.012 | , | | |
| | $\begin{array}{c} 0.002203 \\ -0.02093 \\ 53.61 \\ 0.0135 \\ \hline 0.004796 \\ 0.05756 \\ 0.02981 \\ 7.326 \\ 2.457 \\ 0.305 \\ 0.02136 \\ 0.4862 \\ \hline NO \\ 0.01211 \\ 0.01483 \\ 0.05139 \\ 0.07833 \\ 0.01201 \\ \pm 1.641 \\ \pm 0.3464 \\ \pm 1.254 \\ \end{array}$ | $\begin{array}{c c} \pm 0.09922 & \pm (0.0961 - 0.1027) \\ 1.016 & 1.015 - 1.017 \\ 9.348 & 8.426 - 11.02 \\ 0.002203 & 0.002046 - 0.00236 \\ -0.02093 & -(0.01846 - 0.02363) \\ 53.61 & & & \\ 0.0135 & & & \\ 0.004796 & 0.004454 - 0.005135 \\ 0.05756 & 0.0488 - 0.06388 \\ 0.02981 & 0.02856 - 0.0312 \\ 7.326 & 7.109 - 7.551 \\ 2.457 & 2.421 - 2.489 \\ 0.305 & 0.2825 - 0.3281 \\ 0.02136 & 0.02012 - 0.02282 \\ 0.4862 & 0.4848 - 0.4873 \\ NO & & \\ 0.01211 & 0.01195 - 0.01226 \\ 0.01483 & 0.01477 - 0.01489 \\ 0.05139 & 0.051 - 0.05172 \\ 0.07833 & 0.07774 - 0.07886 \\ 0.01201 & 0.01187 - 0.01213 \\ \pm 1.641 & \pm (1.633 - 1.651) \\ \pm 0.3464 & \pm (0.3335 - 0.3618) \\ \pm 1.254 & \pm (1.238 - 1.271) \\ \end{array}$ | |

Table 1. Best fit values along with 2σ and 3σ ranges of the parameters and observables in the minimal CP-invariant modular S_4 model. CP symmetry is spontaneously broken by the VEV of the modulus τ .

Re τ .¹¹ The three real parameters $v_d \alpha$, β/α and γ/α are fixed by fitting the three charged lepton masses. The remaining three real parameters $v_u^2 g^2/\Lambda$, g'/g, Im τ and the phase Re τ describe the nine neutrino observables: three neutrino masses, three neutrino mixing angles and three CPV phases.

As a result, this model has more predictive power than the original model from ref. [31], which is described by the same parameters and an additional phase $\arg(g'/g)$. In fact, the correlations between $\sin^2 \theta_{23}$, the neutrino masses and the CPV phases, which were present in the original model, now reduce to accurate predictions of these observables at a few percent level. This can be seen by comparing the ranges from table 1 of the present article with table 5a and figure 2 of ref. [31]. Apart from that, many correlations between pairs of observables and between observables and parameters arise. We report these correlations in figures 1 and 2.

¹¹Re τ should be treated as a phase since the dependence of Yukawa couplings and fermion mass matrices on τ arises through powers of $\exp(2\pi i \tau/N) = \exp(\pi i \tau/2)$.

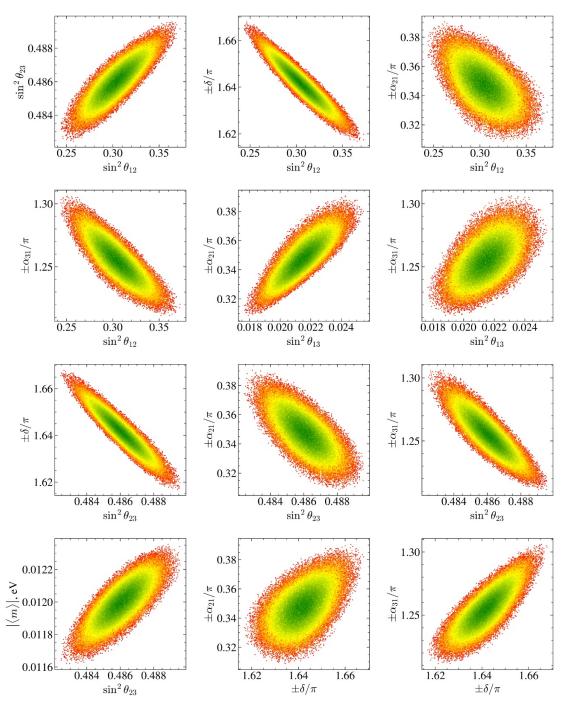


Figure 1. Correlations between pairs of observables in the minimal CP-invariant modular S_4 model.

We also check numerically that CP invariance is restored for the CP-conserving values of τ derived in subsection 4.3. To achieve this, we vary the value of τ while keeping all other parameters fixed to their best fit values, and present the resulting $\sin^2 \delta(\tau)$, $\sin^2 \alpha_{21}(\tau)$ and $\sin^2 \alpha_{31}(\tau)$ as heatmap plots in the τ plane in figure 3. Notice that this variation is done for illustrative purposes only, as it spoils the values of the remaining observables. Those are

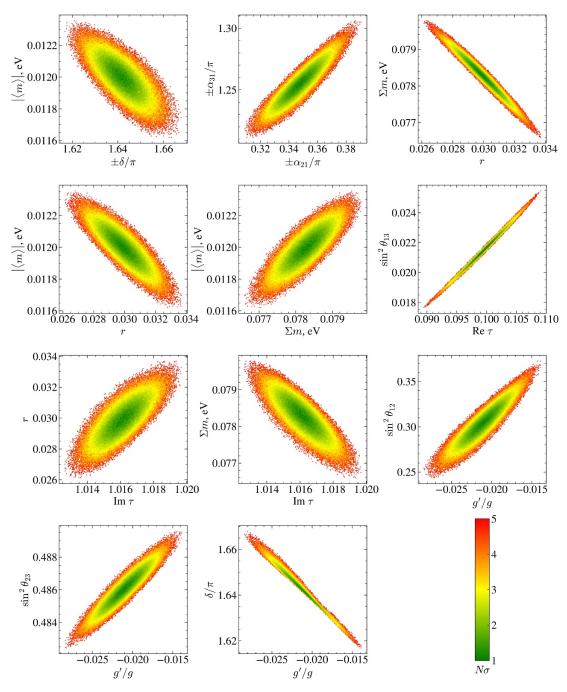


Figure 2. Correlations between pairs of observables (continued from figure 1) and between observables and parameters in the minimal CP-invariant modular S_4 model.

in agreement with experimental data only in a small region of the τ plane [31]. The sinesquared of a phase measures the strength of CPV, with the value of 0 (shown with green colour) corresponding to no CPV and the value of 1 (shown with red colour) corresponding to maximal CPV. As anticipated, both the boundary of \mathcal{D} and the imaginary axis conserve CP, appearing in green colour in figure 3. However, even a small departure from a CP-

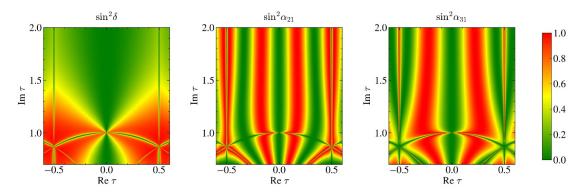


Figure 3. CP violation strength, measured as sine-squared of the CPV phases, for different values of the modulus τ . The boundary of the fundamental domain \mathcal{D} defined in eq. (4.23) and the imaginary axis Re $\tau = 0$ conserve CP. The ranges of Re τ and Im τ are chosen to extend slightly beyond the fundamental domain \mathcal{D} to make its boundary clearly visible.

conserving value of τ can lead to large CPV due to strong dependence of the observables on τ . This is noticeably the case in the vicinity of the boundary of the fundamental domain.

6 Summary and conclusions

In the present article we have developed the formalism of combining modular and generalised CP (gCP) symmetries for theories of flavour. To this end the corresponding consistency conditions for the two symmetry transformations acting on the modulus τ and on the matter fields were derived. We have shown that these consistency conditions imply that under the CP transformation the modulus $\tau \to n - \tau^*$ with integer n, and one can choose n = 0 without loss of generality. This transformation extends the modular group $\overline{\Gamma} \simeq \mathrm{PSL}(2,\mathbb{Z})$ to $\overline{\Gamma}^* \simeq \overline{\Gamma} \rtimes \mathbb{Z}_2^{\mathrm{CP}} \simeq \mathrm{PGL}(2,\mathbb{Z})$. Considering the cases of the finite modular groups Γ_N with N = 2, 3, 4, 5, which are isomorphic to the non-Abelian discrete groups S_3 , A_4 , S_4 and A_5 , respectively, we have demonstrated that the gCP transformation matrix $X_{\mathbf{r}}$ realising a rotation in flavour space when acting on a multiplet $\psi(x)$ as $\psi(x) \to X_{\mathbf{r}} \overline{\psi}(x_P)$, where $x_P = (t, -\mathbf{x})$, can always be chosen to be the identity matrix $\mathbb{1}_{\mathbf{r}}$. Assuming this choice and a proper normalisation of multiplets of modular forms $Y(\tau)$, transforming in irreducible representations of the groups Γ_N with N = 2, 3, 4, 5, we have shown that under CP these multiplets get complex conjugated. As a consequence, we have found that gCP invariance implies that the constants g, which accompany each invariant singlet in the superpotential, must be real. Thus, the number of free parameters in modular-invariant models which also enjoy a gCP symmetry gets reduced, leading to a higher predictive power of such models. In these models, the only source of both modular symmetry breaking and CP violation is the VEV of the modulus τ . We have further demonstrated that CP is conserved for the values of the modulus at the boundary of the fundamental domain and on the imaginary axis.

Finally, via the example of a modular S_4 model of lepton flavour with type I seesaw mechanism of neutrino mass generation, we have illustrated the results obtained in the present study regarding the implications of gCP symmetry in modular-invariant theories of flavour. This model was considered in ref. [31] without the requirement of gCP invariance. We have shown that imposing the latter leads to much reduced ranges of allowed values of the neutrino mass and mixing parameters as well as to much stronger correlations between the different neutrino-related observables (table 1 and figures 1 and 2).

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A Spinors and superfields under CP

For clarity, in this appendix alone chiral superfields will be denoted with a tilde to distinguish them from scalar and fermion fields. Under CP, a 4-component spin-1/2 flavour multiplet Ψ transforms as

$$\Psi_i(x) \xrightarrow{\text{CP}} i (X_{\Psi})_{ij} \gamma^0 C \overline{\Psi_j}^T(x_P), \qquad (A.1)$$

where $x = (t, \mathbf{x}), x_P = (t, -\mathbf{x}), X_{\Psi}$ is a unitary matrix in flavour space and C is the charge conjugation matrix, satisfying $C^{-1}\gamma_{\mu}C = -\gamma_{\mu}^{T}$, which implies $C^{T} = -C$. These two properties of C do not depend on the representation of the γ -matrices. We can further consider C to be unitary, $C^{-1} = C^{\dagger}$, without loss of generality. The factor of i in eq. (A.1) is a convention employed consistently throughout this appendix. Spacetime coordinates are henceforth omitted. For the two-component formalism widely used in SUSY we are going to discuss in the present appendix it proves convenient to consider the Weyl basis for γ^{μ} matrices. In this basis, the matrix C is real, so that $C = -C^{\dagger} = -C^{-1}$.

One may write a 4-component spinor Ψ in terms of two Weyl 2-spinors,

$$\Psi = \begin{pmatrix} \psi_{\alpha} \\ \overline{\phi}^{\dot{\alpha}} \end{pmatrix}, \qquad \Psi^{c} \equiv C \,\overline{\Psi}^{T} = \begin{pmatrix} \phi_{\alpha} \\ \overline{\psi}^{\dot{\alpha}} \end{pmatrix}, \tag{A.2}$$

with dotted and undotted indices shown explicitly. Bars on 2-spinors denote conjugation, e.g. $\overline{\psi}^{\dot{\alpha}} = \delta^{\dot{\alpha}}{}_{\alpha}(\psi^{\alpha})^*$. Notice that for 4-spinors $\overline{\Psi} \equiv \Psi^{\dagger}A$, with A numerically equal to γ^0 but with a different index structure. One has:

$$A = \begin{pmatrix} 0 & \delta^{\alpha}{}_{\dot{\beta}} \\ \delta_{\dot{\alpha}}{}^{\beta} & 0 \end{pmatrix}, \qquad C = \begin{pmatrix} \epsilon_{\alpha\beta} & 0 \\ 0 & \epsilon^{\dot{\alpha}\dot{\beta}} \end{pmatrix}, \quad \text{with } \epsilon^{\dot{\alpha}\dot{\beta}} = -\epsilon_{\alpha\beta} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{A.3}$$

$$\gamma^{\mu} = \begin{pmatrix} 0 & (\sigma^{\mu})_{\alpha\dot{\beta}} \\ (\overline{\sigma}^{\mu})^{\dot{\alpha}\beta} & 0 \end{pmatrix} \quad \Rightarrow \quad \gamma^{0} = \begin{pmatrix} 0 & (\sigma^{0})_{\alpha\dot{\beta}} \\ (\overline{\sigma}^{0})^{\dot{\alpha}\beta} & 0 \end{pmatrix}.$$
(A.4)

Disregarding the spinor-index structure, one has $C = i\gamma^0\gamma^2$, $\gamma^1 = i\gamma^0\gamma^1\gamma^2\gamma^3 = diag(-1, 1)$, $\sigma^{\mu} = (\sigma^0, \sigma^i) = (\sigma_0, -\sigma_i)$ and $\overline{\sigma}^{\mu} = (\sigma_0, \sigma_i)$, with $\sigma_0 = 1$ and the σ_i being the Pauli matrices. The chiral projection operators are defined as $P_{L,R} = (1 \mp \gamma^5)/2$.

From the CP transformation (A.1) of a 4-spinor Ψ , one can obtain the CP transformation of the Weyl spinors ψ and ϕ in eq. (A.2):

$$\psi_{i\alpha} \xrightarrow{\mathrm{CP}} i \left(X_{\Psi} \right)_{ij} \left(\sigma^0 \right)_{\alpha\dot{\beta}} \overline{\psi}_{j}^{\dot{\beta}} \qquad \Rightarrow \qquad \overline{\psi}_{i}^{\dot{\alpha}} \xrightarrow{\mathrm{CP}} i \left(X_{\Psi} \right)_{ij}^* \left(\overline{\sigma}^0 \right)^{\dot{\alpha}\beta} \psi_{j\beta} \,, \tag{A.5}$$

$$\overline{\phi}_{i}^{\dot{\alpha}} \xrightarrow{\mathrm{CP}} i \left(X_{\Psi} \right)_{ij} \left(\overline{\sigma}^{0} \right)^{\dot{\alpha}\beta} \phi_{j\beta} \qquad \Rightarrow \qquad \phi_{i\alpha} \xrightarrow{\mathrm{CP}} i \left(X_{\Psi} \right)_{ij}^{*} \left(\sigma^{0} \right)_{\alpha\dot{\beta}} \overline{\phi}_{j}^{\beta}. \tag{A.6}$$

For the (chiral) fields in the lepton sector, in particular, one has:

$$\ell_{iL} \equiv \begin{pmatrix} L_{i\alpha} \\ 0 \end{pmatrix} \xrightarrow{\text{CP}} i \ (X_L)_{ij} \ \gamma^0 C \ \overline{\ell_{jL}}^T \qquad \Rightarrow \qquad L_{i\alpha} \xrightarrow{\text{CP}} i \ (X_L)_{ij} \ (\sigma^0)_{\alpha\dot{\beta}} \ \overline{L_j}^{\dot{\beta}}, \quad (A.7)$$

$$e_{iR} \equiv \begin{pmatrix} 0 \\ \overline{E_i^{c\dot{\alpha}}} \end{pmatrix} \xrightarrow{\mathrm{CP}} i (X_R)_{ij} \gamma^0 C \overline{e_{jR}}^T \quad \Rightarrow \quad E_{i\,\alpha}^c \xrightarrow{\mathrm{CP}} i (X_R)_{ij}^* (\sigma^0)_{\alpha\dot{\beta}} \overline{E_j^{c\dot{\beta}}}, \quad (A.8)$$

$$\nu_{iR} \equiv \begin{pmatrix} 0\\ \overline{N_i^c}^{\dot{\alpha}} \end{pmatrix} \xrightarrow{\mathrm{CP}} i \ (X_N)_{ij} \ \gamma^0 C \ \overline{\nu_{jR}}^T \quad \Rightarrow \qquad N_{i\alpha}^c \xrightarrow{\mathrm{CP}} i \ (X_N)_{ij}^* \ (\sigma^0)_{\alpha\dot{\beta}} \ \overline{N_j^c}^{\dot{\beta}}, \quad (A.9)$$

where ℓ_{iL} , e_{iR} and ν_{iR} (L_i , E_i^c and N_i^c) denote lepton doublet, charged lepton singlet and neutrino singlet 4(2)-spinors, respectively. It is then straightforward to find the transformation of a pair of contracted spinors, e.g.:

$$E_{i}^{c}L_{j} = \epsilon^{\alpha\beta}E_{i\beta}^{c}L_{j\alpha} \xrightarrow{\text{CP}} (X_{R})_{ik}^{*}(X_{L})_{jl} \left[-(\sigma^{0T})_{\dot{\beta}\alpha}\epsilon^{\alpha\beta}(\sigma^{0})_{\beta\dot{\alpha}} \right] \overline{E_{k}^{c}}^{\dot{\alpha}}\overline{L_{l}}^{\dot{\beta}}$$

$$= (X_{R})_{ik}^{*}(X_{L})_{jl}\overline{E_{k}^{c}}\overline{L_{l}}.$$
(A.10)

In the framework of rigid $\mathcal{N} = 1$ SUSY in 4 dimensions, taking the Graßmann coordinates θ_{α} and $\overline{\theta}^{\dot{\alpha}}$ to transform under CP as all other Weyl spinors, i.e.

$$\theta_{\alpha} \xrightarrow{\mathrm{CP}} i (\sigma^{0})_{\alpha \dot{\beta}} \overline{\theta}^{\dot{\beta}} \quad \Rightarrow \quad \overline{\theta}^{\dot{\alpha}} \xrightarrow{\mathrm{CP}} i (\overline{\sigma}^{0})^{\dot{\alpha}\beta} \theta_{\beta} , \qquad (A.11)$$

one can obtain a consistent CP transformation of a chiral superfield $\tilde{\psi} = \varphi + \sqrt{2} \theta \psi - \theta^2 F$, with F being an auxiliary field and φ denoting the scalar lowest component of the superfield, expected to transform under CP in the same way as the latter. Indeed, using eqs. (A.11) and (A.5), one sees that consistency implies

$$\widetilde{\psi}_i \xrightarrow{\text{CP}} (X_{\Psi})_{ij} \overline{\widetilde{\psi}}_j,$$
(A.12)

¹²The matrix $C = i\gamma^0 \gamma^2$ has the same form in the usual Dirac representation of γ -matrices.

with $\varphi_i \xrightarrow{\text{CP}} (X_{\Psi})_{ij} \varphi_j^*$ and $F_i \xrightarrow{\text{CP}} (X_{\Psi})_{ij} F_j^*$, since $\theta^2 \xrightarrow{\text{CP}} \overline{\theta}^2$, and where the bar denotes the Hermitian conjugated superfield. We thus see that the superpotential, up to unitary rotations in flavour space, is exchanged under CP with its conjugate.¹³

Given the CP transformations of spinors in eqs. (A.7) – (A.9), one then has, for the chiral superfields \widetilde{L}_i , \widetilde{E}_i^c and \widetilde{N}_i^c in the lepton sector:

$$\widetilde{L}_i \xrightarrow{\text{CP}} (X_L)_{ij} \overline{\widetilde{L}}_j \implies \overline{\widetilde{L}}_i \xrightarrow{\text{CP}} (X_L)_{ij}^* \widetilde{L}_j,$$
(A.13)

$$\widetilde{E}_{i}^{c} \xrightarrow{\mathrm{CP}} (X_{R})_{ij}^{*} \overline{\widetilde{E}}_{j}^{c} \Longrightarrow \widetilde{\widetilde{E}}_{i}^{c} \xrightarrow{\mathrm{CP}} (X_{R})_{ij} \widetilde{E}_{j}^{c}, \qquad (A.14)$$

$$\widetilde{N}_{i}^{c} \xrightarrow{\mathrm{CP}} (X_{N})_{ij}^{*} \overline{\widetilde{N}}_{j}^{c} \implies \widetilde{\overline{N}}_{i}^{c} \xrightarrow{\mathrm{CP}} (X_{N})_{ij} \widetilde{N}_{j}^{c}.$$
 (A.15)

B Group theory of $\Gamma_{N<5}$

B.1 Order and irreducible representations

The finite modular groups $\Gamma_N = \overline{\Gamma}/\overline{\Gamma}(N) \simeq \text{PSL}(2,\mathbb{Z}_N)$, with N > 1, can be defined by two generators S and T satisfying the relations:

$$S^2 = T^N = (ST)^3 = I.$$
 (B.1)

The order of these groups is given by (see, e.g., [46]):

$$|\Gamma_N| = \begin{cases} 6 & \text{for } N = 2, \\ \frac{N^3}{2} \prod_{p|N} \left(1 - \frac{1}{p^2} \right) & \text{for } N > 2, \end{cases}$$
(B.2)

where the product is over prime divisors p of N.

It is straightforward to show that $|\Gamma_N|$ is even for all N. Decomposing N > 2 in its unique prime factorisation, $N = \prod_{i=1}^k p_i^{n_i}$ with $n_i \ge 1$, one has:

$$2|\Gamma_{N>2}| = N \prod_{i=1}^{k} p_i^{2(n_i-1)} \left(p_i^2 - 1\right).$$
(B.3)

The group order will be even if $2|\Gamma_{N>2}|$ is a multiple of 4. This is trivially verified when N is a power of 2. If N is not a power of 2, then at least one of its prime factors is odd, say p_j . Since $(n^2 - 1) \equiv 0 \pmod{4}$ for odd n, it follows that the group order is even also in this case, as $(p_j^2 - 1)$ divides $2|\Gamma_{N>2}|$.

In what follows, we focus on the case $N \leq 5$. The orders and irreducible representations of these groups are listed in table 2.

B.2 Symmetric basis for group generators

For the groups S_3 , A_4 , S_4 and A_5 , we explicitly give below the basis for representation matrices in which the group generators S and T are represented by symmetric matrices, see eq. (2.11), for all irreducible representations **r** (see, e.g., refs. [2, 21, 47, 48]).

¹³One can check that the Graßmann integration $\int d^2\theta$ is exchanged with its conjugate $\int d^2\overline{\theta}$.

| Γ_N | $\Gamma_2 \simeq S_3$ | $\Gamma_3 \simeq A_4$ | $\Gamma_4 \simeq S_4$ | $\Gamma_5 \simeq A_5$ |
|--------------|---------------------------------|--|---|-----------------------|
| $ \Gamma_N $ | 6 | 12 | 24 | 60 |
| irreps | 1 , 1 ', 2 | 1 , 1 ', 1 '', 3 | ${\bf 1}, {\bf 1}', {\bf 2}, {\bf 3}, {\bf 3}'$ | ${f 1,3,3',4,5}$ |

Table 2. Orders and irreducible representations for finite modular groups Γ_N with $N \leq 5$.

B.2.1 $\Gamma_2 \simeq S_3$

1:
$$\rho(S) = 1$$
, $\rho(T) = 1$, (B.4)

1':
$$\rho(S) = -1,$$
 $\rho(T) = -1,$ (B.5)

:
$$\rho(S) = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}, \qquad \rho(T) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
 (B.6)

B.2.2 $\Gamma_3 \simeq A_4$

 $\mathbf{2}$

1:
$$\rho(S) = 1$$
, $\rho(T) = 1$, (B.7)

1':
$$\rho(S) = 1,$$
 $\rho(T) = \omega,$ (B.8)

1":
$$\rho(S) = 1,$$
 $\rho(T) = \omega^2,$ (B.9)

3:
$$\rho(S) = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}, \qquad \rho(T) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \qquad (B.10)$$

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

B.2.3 $\Gamma_4\simeq S_4$

1: $\rho(S) = 1$, $\rho(T) = 1$, (B.11)

1':
$$\rho(S) = -1,$$
 $\rho(T) = -1,$ (B.12)

2:
$$\rho(S) = \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \qquad \rho(T) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (B.13)$$

$$\mathbf{3}: \qquad \rho(S) = -\frac{1}{2} \begin{pmatrix} 0 & \sqrt{2} & \sqrt{2} \\ \sqrt{2} & -1 & 1 \\ \sqrt{2} & 1 & -1 \end{pmatrix}, \qquad \rho(T) = -\begin{pmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -i \end{pmatrix}, \qquad (B.14)$$

$$\mathbf{3}': \qquad \rho(S) = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{2} & \sqrt{2} \\ \sqrt{2} & -1 & 1 \\ \sqrt{2} & 1 & -1 \end{pmatrix}, \qquad \rho(T) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -i \end{pmatrix}. \tag{B.15}$$

B.2.4 $\Gamma_5 \simeq A_5$

1:
$$\rho(S) = 1$$
, $\rho(T) = 1$, (B.16)

$$\mathbf{3}: \qquad \rho(S) = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & -\sqrt{2} & -\sqrt{2} \\ -\sqrt{2} & -\varphi & 1/\varphi \\ -\sqrt{2} & 1/\varphi & -\varphi \end{pmatrix}, \qquad \qquad \rho(T) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \zeta & 0 \\ 0 & 0 & \zeta^4 \end{pmatrix}, \qquad (B.17)$$

$$\mathbf{3}': \qquad \rho(S) = \frac{1}{\sqrt{5}} \begin{pmatrix} -1 & \sqrt{2} & \sqrt{2} \\ \sqrt{2} & -1/\varphi & \varphi \\ \sqrt{2} & \varphi & -1/\varphi \end{pmatrix}, \qquad \qquad \rho(T) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \zeta^2 & 0 \\ 0 & 0 & \zeta^3 \end{pmatrix}, \qquad (B.18)$$

$$\begin{aligned}
\mathbf{4}: \quad \rho(S) &= \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 1/\varphi & \varphi & -1 \\ 1/\varphi & -1 & 1 & \varphi \\ \varphi & 1 & -1 & 1/\varphi \\ -1 & \varphi & 1/\varphi & 1 \end{pmatrix}, \qquad \rho(T) = \begin{pmatrix} \zeta & 0 & 0 & 0 \\ 0 & \zeta^2 & 0 & 0 \\ 0 & 0 & \zeta^3 & 0 \\ 0 & 0 & 0 & \zeta^4 \end{pmatrix}, \quad (B.19) \\
\mathbf{5}: \quad \rho(S) &= \frac{1}{5} \begin{pmatrix} -1 & \sqrt{6} & \sqrt{6} & \sqrt{6} & \sqrt{6} \\ \sqrt{6} & 1/\varphi^2 & -2\varphi & 2/\varphi & \varphi^2 \\ \sqrt{6} & -2\varphi & \varphi^2 & 1/\varphi^2 & 2/\varphi \\ \sqrt{6} & 2/\varphi & 1/\varphi^2 & \varphi^2 & -2\varphi \\ \sqrt{6} & \varphi^2 & 2/\varphi & -2\varphi & 1/\varphi^2 \end{pmatrix}, \qquad \rho(T) = \begin{pmatrix} \zeta & 0 & 0 & 0 \\ 0 & \zeta^2 & 0 & 0 \\ 0 & 0 & \zeta^2 & 0 & 0 \\ 0 & 0 & 0 & \zeta^4 \end{pmatrix}, \quad (B.20)
\end{aligned}$$

where $\zeta = e^{2\pi i/5}$ and $\varphi = (1 + \sqrt{5})/2$.

B.3 Clebsch-Gordan coefficients

For completeness, and for each level N = 2, 3, 4, 5, we also reproduce here the nontrivial Clebsch-Gordan coefficients in the symmetric basis of appendix B.2. Entries of each multiplet entering the tensor product are denoted by α_i and β_i .

B.3.1 $\Gamma_2 \simeq S_3$

B.3.2 $\Gamma_3 \simeq A_4$

$$\mathbf{1}' \otimes \mathbf{1}' = \mathbf{1}'' \quad \sim \quad \alpha_1 \beta_1$$
$$\mathbf{1}'' \otimes \mathbf{1}'' = \mathbf{1}' \quad \sim \quad \alpha_1 \beta_1$$

$$\begin{split} \mathbf{1}' \otimes \mathbf{1}'' &= \mathbf{1} & \sim & \alpha_1 \, \beta_1 \\ \mathbf{1}' \otimes \mathbf{3} &= \mathbf{3} & \sim & \begin{pmatrix} \alpha_1 \, \beta_3 \\ \alpha_1 \, \beta_1 \\ \alpha_1 \, \beta_2 \end{pmatrix} \\ \mathbf{1}'' \otimes \mathbf{3} &= \mathbf{3} & \sim & \begin{pmatrix} \alpha_1 \, \beta_2 \\ \alpha_1 \, \beta_3 \\ \alpha_1 \, \beta_1 \end{pmatrix} \\ \mathbf{3} \otimes \mathbf{3} &= \mathbf{1} \oplus \mathbf{1}' \oplus \mathbf{1}'' \oplus \mathbf{3}_1 \oplus \mathbf{3}_2 \end{split}$$

$$\left\{\begin{array}{cccc} \mathbf{1} & \sim & \alpha_1\beta_1 + \alpha_2\beta_3 + \alpha_3\beta_2 \\ \mathbf{1}' & \sim & \alpha_1\beta_2 + \alpha_2\beta_1 + \alpha_3\beta_3 \\ \mathbf{1}'' & \sim & \alpha_1\beta_3 + \alpha_2\beta_2 + \alpha_3\beta_1 \\ \mathbf{3}_1 & \sim & \begin{pmatrix} 2\alpha_1\beta_1 - \alpha_2\beta_3 - \alpha_3\beta_2 \\ 2\alpha_3\beta_3 - \alpha_1\beta_2 - \alpha_2\beta_1 \\ 2\alpha_2\beta_2 - \alpha_3\beta_1 - \alpha_1\beta_3 \end{pmatrix} \\ \mathbf{3}_2 & \sim & \begin{pmatrix} \alpha_2\beta_3 - \alpha_3\beta_2 \\ \alpha_1\beta_2 - \alpha_2\beta_1 \\ \alpha_3\beta_1 - \alpha_1\beta_3 \end{pmatrix} \end{array}\right\}$$

B.3.3 $\Gamma_4\simeq S_4$

$$\begin{split} \mathbf{1}' \otimes \mathbf{1}' &= \mathbf{1} &\sim & \alpha_1 \,\beta_1 \\ \mathbf{1}' \otimes \mathbf{2} &= \mathbf{2} &\sim & \begin{pmatrix} \alpha_1 \,\beta_2 \\ -\alpha_1 \,\beta_1 \end{pmatrix} \\ \mathbf{1}' \otimes \mathbf{3} &= \mathbf{3}' &\sim & \begin{pmatrix} \alpha_1 \,\beta_1 \\ \alpha_1 \,\beta_2 \\ \alpha_1 \,\beta_3 \end{pmatrix} \\ \mathbf{1}' \otimes \mathbf{3}' &= \mathbf{3} &\sim & \begin{pmatrix} \alpha_1 \,\beta_1 \\ \alpha_1 \,\beta_2 \\ \alpha_1 \,\beta_3 \end{pmatrix} \\ \mathbf{2} \otimes \mathbf{2} &= \mathbf{1} \oplus \mathbf{1}' \oplus \mathbf{2} \\ & \begin{cases} \mathbf{1} &\sim & \alpha_1 \beta_1 + \alpha_2 \beta_2 \\ \mathbf{1}' &\sim & \alpha_1 \beta_2 - \alpha_2 \beta_1 \\ \mathbf{2} &\sim & \begin{pmatrix} \alpha_2 \,\beta_2 - \alpha_1 \,\beta_1 \\ \alpha_1 \,\beta_2 + \alpha_2 \,\beta_1 \end{pmatrix} \end{cases}$$

 $\mathbf{2}\,\otimes\,\mathbf{3}\,=\,\mathbf{3}\,\oplus\,\mathbf{3}'$

$$\begin{cases} \mathbf{3} \sim \begin{pmatrix} \alpha_1 \, \beta_1 \\ (\sqrt{3}/2) \, \alpha_2 \, \beta_3 - (1/2) \, \alpha_1 \, \beta_2 \\ (\sqrt{3}/2) \, \alpha_2 \, \beta_2 - (1/2) \, \alpha_1 \, \beta_3 \end{pmatrix} \\ \mathbf{3'} \sim \begin{pmatrix} -\alpha_2 \, \beta_1 \\ (\sqrt{3}/2) \, \alpha_1 \, \beta_3 + (1/2) \, \alpha_2 \, \beta_2 \\ (\sqrt{3}/2) \, \alpha_1 \, \beta_2 + (1/2) \, \alpha_2 \, \beta_3 \end{pmatrix} \end{cases}$$

 $\begin{array}{l} \mathbf{2} \,\otimes\, \mathbf{3}' \,=\, \mathbf{3} \,\oplus\, \mathbf{3}' \\ \left\{ \begin{array}{ccc} \mathbf{3} &\sim & \begin{pmatrix} -\alpha_2\,\beta_1 \\ (\sqrt{3}/2)\,\alpha_1\,\beta_3 + (1/2)\,\alpha_2\,\beta_2 \\ (\sqrt{3}/2)\,\alpha_1\,\beta_2 + (1/2)\,\alpha_2\,\beta_3 \end{pmatrix} \\ \mathbf{3}' &\sim & \begin{pmatrix} \alpha_1\,\beta_1 \\ (\sqrt{3}/2)\,\alpha_2\,\beta_3 - (1/2)\,\alpha_1\,\beta_2 \\ (\sqrt{3}/2)\,\alpha_2\,\beta_2 - (1/2)\,\alpha_1\,\beta_3 \end{pmatrix} \end{array} \right. \end{array}$

 $\mathbf{3} \otimes \mathbf{3} = \mathbf{3}' \otimes \mathbf{3}' = \mathbf{1} \oplus \mathbf{2} \oplus \mathbf{3} \oplus \mathbf{3}'$ $\begin{cases} \mathbf{1} \sim \alpha_1 \beta_1 + \alpha_2 \beta_3 + \alpha_3 \beta_2 \\ \mathbf{2} \sim \begin{pmatrix} \alpha_1 \beta_1 - (1/2) (\alpha_2 \beta_3 + \alpha_3 \beta_2) \\ (\sqrt{3}/2) (\alpha_2 \beta_2 + \alpha_3 \beta_3) \end{pmatrix} \\ \mathbf{3} \sim \begin{pmatrix} \alpha_3 \beta_3 - \alpha_2 \beta_2 \\ \alpha_1 \beta_3 + \alpha_3 \beta_1 \\ -\alpha_1 \beta_2 - \alpha_2 \beta_1 \end{pmatrix} \\ \mathbf{3}' \sim \begin{pmatrix} \alpha_3 \beta_2 - \alpha_2 \beta_3 \\ \alpha_2 \beta_1 - \alpha_1 \beta_2 \\ \alpha_1 \beta_3 - \alpha_3 \beta_1 \end{pmatrix}$

 $\mathbf{3}\,\otimes\,\mathbf{3}'\,=\,\mathbf{1}'\,\oplus\,\mathbf{2}\,\oplus\,\mathbf{3}\,\oplus\,\mathbf{3}'$

$$\begin{array}{rcl}
 1' & \sim & \alpha_1\beta_1 + \alpha_2\beta_3 + \alpha_3\beta_2 \\
 2 & \sim & \left((\sqrt{3}/2) \left(\alpha_2\beta_2 + \alpha_3\beta_3 \right) \\
 -\alpha_1\beta_1 + (1/2) \left(\alpha_2\beta_3 + \alpha_3\beta_2 \right) \right) \\
 3 & \sim & \left(\begin{array}{c} \alpha_3\beta_2 - \alpha_2\beta_3 \\ \alpha_2\beta_1 - \alpha_1\beta_2 \\ \alpha_1\beta_3 - \alpha_3\beta_1 \end{array} \right) \\
 3' & \sim & \left(\begin{array}{c} \alpha_3\beta_3 - \alpha_2\beta_2 \\ \alpha_1\beta_3 + \alpha_3\beta_1 \\ -\alpha_1\beta_2 - \alpha_2\beta_1 \end{array} \right) \\
 \end{array}$$

B.3.4 $\Gamma_5 \simeq A_5$

3

 $\mathbf{3}\,\otimes\,\mathbf{3}'\,=\,\mathbf{4}\,\oplus\,\mathbf{5}$

$$4 \sim \begin{pmatrix} \sqrt{2} \alpha_2 \beta_1 + \alpha_3 \beta_2 \\ -\sqrt{2} \alpha_1 \beta_2 - \alpha_3 \beta_3 \\ -\sqrt{2} \alpha_1 \beta_3 - \alpha_2 \beta_2 \\ \sqrt{2} \alpha_3 \beta_1 + \alpha_2 \beta_3 \end{pmatrix}$$
$$5 \sim \begin{pmatrix} \sqrt{3} \alpha_1 \beta_1 \\ \alpha_2 \beta_1 - \sqrt{2} \alpha_3 \beta_2 \\ \alpha_1 \beta_2 - \sqrt{2} \alpha_3 \beta_3 \\ \alpha_1 \beta_3 - \sqrt{2} \alpha_2 \beta_2 \\ \alpha_3 \beta_1 - \sqrt{2} \alpha_2 \beta_3 \end{pmatrix}$$

$$\mathbf{3}\,\otimes\,\mathbf{4}\,=\,\mathbf{3}'\,\oplus\,\mathbf{4}\,\oplus\,\mathbf{5}$$

$$\begin{cases} \mathbf{3'} \sim \begin{pmatrix} -\sqrt{2} \alpha_2 \beta_4 - \sqrt{2} \alpha_3 \beta_1 \\ \sqrt{2} \alpha_1 \beta_2 - \alpha_2 \beta_1 + \alpha_3 \beta_3 \\ \sqrt{2} \alpha_1 \beta_3 + \alpha_2 \beta_2 - \alpha_3 \beta_4 \end{pmatrix} \\ \mathbf{4} \sim \begin{pmatrix} \alpha_1 \beta_1 - \sqrt{2} \alpha_3 \beta_2 \\ -\alpha_1 \beta_2 - \sqrt{2} \alpha_2 \beta_1 \\ \alpha_1 \beta_3 + \sqrt{2} \alpha_3 \beta_4 \\ -\alpha_1 \beta_4 + \sqrt{2} \alpha_2 \beta_3 \end{pmatrix} \\ \mathbf{5} \sim \begin{pmatrix} \sqrt{6} \alpha_2 \beta_4 - \sqrt{6} \alpha_3 \beta_1 \\ 2\sqrt{2} \alpha_1 \beta_1 + 2\alpha_3 \beta_2 \\ -\sqrt{2} \alpha_1 \beta_2 + \alpha_2 \beta_1 + 3\alpha_3 \beta_3 \\ \sqrt{2} \alpha_1 \beta_3 - 3\alpha_2 \beta_2 - \alpha_3 \beta_4 \\ -2\sqrt{2} \alpha_1 \beta_4 - 2\alpha_2 \beta_3 \end{pmatrix} \end{cases}$$

 $\mathbf{3}\,\otimes\,\mathbf{5}\,=\,\mathbf{3}\,\oplus\,\mathbf{3}'\,\oplus\,\mathbf{4}\,\oplus\,\mathbf{5}$

$$\begin{cases} \mathbf{3} \sim \begin{pmatrix} -2\alpha_{1}\beta_{1} + \sqrt{3}\,\alpha_{2}\beta_{5} + \sqrt{3}\,\alpha_{3}\beta_{2} \\ \sqrt{3}\,\alpha_{1}\beta_{2} + \alpha_{2}\beta_{1} - \sqrt{6}\,\alpha_{3}\beta_{3} \\ \sqrt{3}\,\alpha_{1}\beta_{5} - \sqrt{6}\,\alpha_{2}\beta_{4} + \alpha_{3}\beta_{1} \end{pmatrix} \\ \mathbf{3'} \sim \begin{pmatrix} \sqrt{3}\,\alpha_{1}\beta_{1} + \alpha_{2}\beta_{5} + \alpha_{3}\beta_{2} \\ \alpha_{1}\beta_{3} - \sqrt{2}\,\alpha_{2}\beta_{2} - \sqrt{2}\,\alpha_{3}\beta_{4} \\ \alpha_{1}\beta_{4} - \sqrt{2}\,\alpha_{2}\beta_{3} - \sqrt{2}\,\alpha_{3}\beta_{5} \end{pmatrix} \\ \mathbf{4} \sim \begin{pmatrix} 2\sqrt{2}\,\alpha_{1}\beta_{2} - \sqrt{6}\,\alpha_{2}\beta_{1} + \alpha_{3}\beta_{3} \\ -\sqrt{2}\,\alpha_{1}\beta_{3} + 2\alpha_{2}\beta_{2} - 3\alpha_{3}\beta_{4} \\ \sqrt{2}\,\alpha_{1}\beta_{4} + 3\alpha_{2}\beta_{3} - 2\alpha_{3}\beta_{5} \\ -2\sqrt{2}\,\alpha_{1}\beta_{5} - \alpha_{2}\beta_{4} + \sqrt{6}\,\alpha_{3}\beta_{1} \end{pmatrix} \\ \mathbf{5} \sim \begin{pmatrix} \sqrt{3}\,\alpha_{2}\beta_{5} - \sqrt{3}\,\alpha_{3}\beta_{2} \\ -\alpha_{1}\beta_{2} - \sqrt{3}\,\alpha_{2}\beta_{1} - \sqrt{2}\,\alpha_{3}\beta_{3} \\ -2\alpha_{1}\beta_{3} - \sqrt{2}\,\alpha_{2}\beta_{2} \\ 2\alpha_{1}\beta_{4} + \sqrt{2}\,\alpha_{3}\beta_{5} \\ \alpha_{1}\beta_{5} + \sqrt{2}\,\alpha_{2}\beta_{4} + \sqrt{3}\,\alpha_{3}\beta_{1} \end{pmatrix} \end{cases}$$

$$\begin{aligned} \mathbf{3}' \,\otimes\, \mathbf{3}' \,=\, \mathbf{1} \,\oplus\, \mathbf{3}' \,\oplus\, \mathbf{5} \\ \left\{ \begin{array}{ccc} \mathbf{1} &\sim & \alpha_1 \beta_1 + \alpha_2 \beta_3 + \alpha_3 \beta_2 \\ \mathbf{3}' &\sim & \begin{pmatrix} \alpha_2 \,\beta_3 - \alpha_3 \,\beta_2 \\ \alpha_1 \,\beta_2 - \alpha_2 \,\beta_1 \\ \alpha_3 \,\beta_1 - \alpha_1 \,\beta_3 \end{pmatrix} \\ & & & \begin{pmatrix} 2\alpha_1 \beta_1 - \alpha_2 \beta_3 - \alpha_3 \beta_2 \\ \sqrt{6} \,\alpha_3 \beta_3 \\ -\sqrt{3} \,\alpha_1 \beta_2 - \sqrt{3} \,\alpha_2 \beta_1 \\ -\sqrt{3} \,\alpha_1 \beta_3 - \sqrt{3} \,\alpha_3 \beta_1 \\ \sqrt{6} \,\alpha_2 \beta_2 \end{pmatrix} \end{aligned} \right. \end{aligned}$$

 $\mathbf{3'} \otimes \mathbf{4} = \mathbf{3} \oplus \mathbf{4} \oplus \mathbf{5}$

$$\begin{cases} \mathbf{3} \sim \begin{pmatrix} -\sqrt{2} \alpha_2 \beta_3 - \sqrt{2} \alpha_3 \beta_2 \\ \sqrt{2} \alpha_1 \beta_1 + \alpha_2 \beta_4 - \alpha_3 \beta_3 \\ \sqrt{2} \alpha_1 \beta_4 - \alpha_2 \beta_2 + \alpha_3 \beta_1 \end{pmatrix} \\ \mathbf{4} \sim \begin{pmatrix} \alpha_1 \beta_1 + \sqrt{2} \alpha_3 \beta_3 \\ \alpha_1 \beta_2 - \sqrt{2} \alpha_3 \beta_4 \\ -\alpha_1 \beta_3 + \sqrt{2} \alpha_2 \beta_1 \\ -\alpha_1 \beta_4 - \sqrt{2} \alpha_2 \beta_2 \end{pmatrix} \\ \mathbf{5} \sim \begin{pmatrix} \sqrt{6} \alpha_2 \beta_3 - \sqrt{6} \alpha_3 \beta_2 \\ \sqrt{2} \alpha_1 \beta_1 - 3 \alpha_2 \beta_4 - \alpha_3 \beta_3 \\ 2\sqrt{2} \alpha_1 \beta_2 + 2 \alpha_3 \beta_4 \\ -2\sqrt{2} \alpha_1 \beta_3 - 2 \alpha_2 \beta_1 \\ -\sqrt{2} \alpha_1 \beta_4 + \alpha_2 \beta_2 + 3 \alpha_3 \beta_1 \end{pmatrix}$$

 $\mathbf{3'} \otimes \mathbf{5} = \mathbf{3} \oplus \mathbf{3'} \oplus \mathbf{4} \oplus \mathbf{5}$

$$\begin{cases} \mathbf{3} \sim \begin{pmatrix} \sqrt{3} \alpha_{1}\beta_{1} + \alpha_{2}\beta_{4} + \alpha_{3}\beta_{3} \\ \alpha_{1}\beta_{2} - \sqrt{2} \alpha_{2}\beta_{5} - \sqrt{2} \alpha_{3}\beta_{4} \\ \alpha_{1}\beta_{5} - \sqrt{2} \alpha_{2}\beta_{3} - \sqrt{2} \alpha_{3}\beta_{2} \end{pmatrix} \\ \mathbf{3'} \sim \begin{pmatrix} -2\alpha_{1}\beta_{1} + \sqrt{3} \alpha_{2}\beta_{4} + \sqrt{3} \alpha_{3}\beta_{3} \\ \sqrt{3} \alpha_{1}\beta_{3} + \alpha_{2}\beta_{1} - \sqrt{6} \alpha_{3}\beta_{5} \\ \sqrt{3} \alpha_{1}\beta_{4} - \sqrt{6} \alpha_{2}\beta_{2} + \alpha_{3}\beta_{1} \end{pmatrix} \\ \mathbf{4} \sim \begin{pmatrix} \sqrt{2} \alpha_{1}\beta_{2} + 3\alpha_{2}\beta_{5} - 2\alpha_{3}\beta_{4} \\ 2\sqrt{2} \alpha_{1}\beta_{3} - \sqrt{6} \alpha_{2}\beta_{1} + \alpha_{3}\beta_{5} \\ -2\sqrt{2} \alpha_{1}\beta_{4} - \alpha_{2}\beta_{2} + \sqrt{6} \alpha_{3}\beta_{1} \\ -\sqrt{2} \alpha_{1}\beta_{5} + 2\alpha_{2}\beta_{3} - 3\alpha_{3}\beta_{2} \end{pmatrix} \\ \mathbf{5} \sim \begin{pmatrix} \sqrt{3} \alpha_{2}\beta_{4} - \sqrt{3}\alpha_{3}\beta_{3} \\ 2\alpha_{1}\beta_{2} + \sqrt{2} \alpha_{3}\beta_{4} \\ -\alpha_{1}\beta_{3} - \sqrt{3} \alpha_{2}\beta_{1} - \sqrt{2} \alpha_{3}\beta_{5} \\ \alpha_{1}\beta_{4} + \sqrt{2} \alpha_{2}\beta_{2} + \sqrt{3} \alpha_{3}\beta_{1} \\ -2\alpha_{1}\beta_{5} - \sqrt{2} \alpha_{2}\beta_{3} \end{pmatrix} \end{cases}$$

 $\mathbf{4}\,\otimes\,\mathbf{4}\,=\,\mathbf{1}\,\oplus\,\mathbf{3}\,\oplus\,\mathbf{3}'\,\oplus\,\mathbf{4}\,\oplus\,\mathbf{5}$

$$\begin{array}{lcl} \mathbf{1} & \sim & \alpha_{1}\beta_{4} + \alpha_{2}\beta_{3} + \alpha_{3}\beta_{2} + \alpha_{4}\beta_{1} \\ \mathbf{3} & \sim & \begin{pmatrix} -\alpha_{1}\beta_{4} + \alpha_{2}\beta_{3} - \alpha_{3}\beta_{2} + \alpha_{4}\beta_{1} \\ \sqrt{2}\alpha_{2}\beta_{4} - \sqrt{2}\alpha_{4}\beta_{2} \\ \sqrt{2}\alpha_{1}\beta_{3} - \sqrt{2}\alpha_{3}\beta_{1} \end{pmatrix} \\ \mathbf{3'} & \sim & \begin{pmatrix} \alpha_{1}\beta_{4} + \alpha_{2}\beta_{3} - \alpha_{3}\beta_{2} - \alpha_{4}\beta_{1} \\ \sqrt{2}\alpha_{3}\beta_{4} - \sqrt{2}\alpha_{4}\beta_{3} \\ \sqrt{2}\alpha_{1}\beta_{2} - \sqrt{2}\alpha_{2}\beta_{1} \end{pmatrix} \\ \mathbf{4} & \sim & \begin{pmatrix} \alpha_{2}\beta_{4} + \alpha_{3}\beta_{3} + \alpha_{4}\beta_{2} \\ \alpha_{1}\beta_{1} + \alpha_{3}\beta_{4} + \alpha_{4}\beta_{3} \\ \alpha_{1}\beta_{2} + \alpha_{2}\beta_{1} + \alpha_{4}\beta_{4} \\ \alpha_{1}\beta_{3} + \alpha_{2}\beta_{2} + \alpha_{3}\beta_{1} \end{pmatrix} \\ \mathbf{5} & \sim & \begin{pmatrix} \sqrt{3}\alpha_{1}\beta_{4} - \sqrt{3}\alpha_{2}\beta_{3} - \sqrt{3}\alpha_{3}\beta_{2} + \sqrt{3}\alpha_{4}\beta_{1} \\ -\sqrt{2}\alpha_{2}\beta_{4} + 2\sqrt{2}\alpha_{3}\beta_{3} - \sqrt{2}\alpha_{4}\beta_{2} \\ -2\sqrt{2}\alpha_{1}\beta_{1} + \sqrt{2}\alpha_{3}\beta_{4} + \sqrt{2}\alpha_{4}\beta_{3} \\ \sqrt{2}\alpha_{1}\beta_{2} + \sqrt{2}\alpha_{2}\beta_{1} - 2\sqrt{2}\alpha_{3}\beta_{1} \end{pmatrix} \end{array}$$

 $\mathbf{4}\,\otimes\,\mathbf{5}\,=\,\mathbf{3}\,\oplus\,\mathbf{3}'\,\oplus\,\mathbf{4}\,\oplus\,\mathbf{5}_1\,\oplus\,\mathbf{5}_2$

$$\begin{array}{lcl} \mathbf{1} & \sim & \alpha_{1}\beta_{1} + \alpha_{2}\beta_{5} + \alpha_{3}\beta_{4} + \alpha_{4}\beta_{3} + \alpha_{5}\beta_{2} \\ \mathbf{3} & \sim & \begin{pmatrix} \alpha_{2}\beta_{5} + 2\alpha_{3}\beta_{4} - 2\alpha_{4}\beta_{3} - \alpha_{5}\beta_{2} \\ -\sqrt{3}\,\alpha_{1}\beta_{2} + \sqrt{3}\,\alpha_{2}\beta_{1} + \sqrt{2}\,\alpha_{3}\beta_{5} - \sqrt{2}\,\alpha_{5}\beta_{3} \\ \sqrt{3}\,\alpha_{1}\beta_{5} + \sqrt{2}\,\alpha_{2}\beta_{4} - \sqrt{2}\,\alpha_{4}\beta_{2} - \sqrt{3}\,\alpha_{5}\beta_{1} \end{pmatrix} \\ \mathbf{3}' & \sim & \begin{pmatrix} 2\alpha_{2}\beta_{5} - \alpha_{3}\beta_{4} + \alpha_{4}\beta_{3} - 2\alpha_{5}\beta_{2} \\ \sqrt{3}\,\alpha_{1}\beta_{3} - \sqrt{3}\,\alpha_{3}\beta_{1} + \sqrt{2}\,\alpha_{4}\beta_{5} - \sqrt{2}\,\alpha_{5}\beta_{4} \\ -\sqrt{3}\,\alpha_{1}\beta_{4} + \sqrt{2}\,\alpha_{2}\beta_{3} - \sqrt{2}\,\alpha_{3}\beta_{2} + \sqrt{3}\,\alpha_{4}\beta_{1} - \sqrt{3}\,\alpha_{5}\beta_{3} \\ 3\sqrt{2}\,\alpha_{1}\beta_{3} + 4\sqrt{3}\,\alpha_{2}\beta_{2} + 3\sqrt{2}\,\alpha_{3}\beta_{1} - \sqrt{3}\,\alpha_{4}\beta_{5} - \sqrt{3}\,\alpha_{5}\beta_{4} \\ 3\sqrt{2}\,\alpha_{1}\beta_{3} + 4\sqrt{3}\,\alpha_{2}\beta_{3} - \sqrt{3}\,\alpha_{3}\beta_{2} + 3\sqrt{2}\,\alpha_{4}\beta_{1} + 4\sqrt{3}\,\alpha_{5}\beta_{5} \\ 3\sqrt{2}\,\alpha_{1}\beta_{5} - \sqrt{3}\,\alpha_{2}\beta_{4} + 4\sqrt{3}\,\alpha_{3}\beta_{5} - \sqrt{3}\,\alpha_{5}\beta_{3} \\ -\sqrt{2}\,\alpha_{1}\beta_{3} + \sqrt{2}\,\alpha_{3}\beta_{1} + \sqrt{3}\,\alpha_{4}\beta_{5} - \sqrt{3}\,\alpha_{5}\beta_{4} \\ -\sqrt{2}\,\alpha_{1}\beta_{4} - \sqrt{3}\,\alpha_{2}\beta_{3} + \sqrt{3}\,\alpha_{3}\beta_{2} + \sqrt{2}\,\alpha_{4}\beta_{1} \\ \sqrt{2}\,\alpha_{1}\beta_{5} - \sqrt{3}\,\alpha_{2}\beta_{4} + \sqrt{3}\,\alpha_{4}\beta_{2} - \sqrt{2}\,\alpha_{5}\beta_{1} \\ \end{pmatrix} \\ \mathbf{5}_{1} & \sim & \begin{pmatrix} 2\alpha_{1}\beta_{1} + \alpha_{2}\beta_{5} - 2\alpha_{3}\beta_{4} - 2\alpha_{4}\beta_{3} + \alpha_{5}\beta_{2} \\ \alpha_{1}\beta_{2} + \alpha_{2}\beta_{1} + \sqrt{6}\,\alpha_{3}\beta_{5} + \sqrt{6}\,\alpha_{5}\beta_{3} \\ -2\alpha_{1}\beta_{4} - 2\alpha_{4}\beta_{1} + \sqrt{6}\,\alpha_{5}\beta_{5} \\ \alpha_{1}\beta_{5} + \sqrt{6}\,\alpha_{2}\beta_{4} + \sqrt{6}\,\alpha_{4}\beta_{2} + \alpha_{5}\beta_{1} \\ \end{pmatrix} \\ \mathbf{5}_{2} & \sim & \begin{pmatrix} 2\alpha_{1}\beta_{1} - 2\alpha_{2}\beta_{5} + \alpha_{3}\beta_{4} + \alpha_{4}\beta_{3} - 2\alpha_{5}\beta_{2} \\ \alpha_{1}\beta_{3} + \alpha_{3}\beta_{1} + \sqrt{6}\,\alpha_{4}\beta_{2} + \alpha_{5}\beta_{1} \\ -2\alpha_{1}\beta_{2} - 2\alpha_{2}\beta_{1} + \sqrt{6}\,\alpha_{3}\beta_{2} + \alpha_{4}\beta_{1} \\ \alpha_{1}\beta_{3} + \alpha_{3}\beta_{1} + \sqrt{6}\,\alpha_{3}\beta_{2} + \alpha_{4}\beta_{1} \\ \alpha_{1}\beta_{4} + \sqrt{6}\,\alpha_{2}\beta_{3} + \sqrt{6}\,\alpha_{3}\beta_{2} + \alpha_{4}\beta_{1} \\ -2\alpha_{1}\beta_{5} + \sqrt{6}\,\alpha_{3}\beta_{3} - 2\alpha_{5}\beta_{1} \\ \end{pmatrix} \end{array}$$

C Modular form multiplets

C.1 Lowest weight multiplets

For the groups Γ_N with $N \leq 5$, the lowest (non-trivial) weight modular multiplets can be constructed from linear combinations $Y(a_i|\tau)$ of logarithmic derivatives of some seed functions. These functions are the Dedekind eta $\eta(\tau)$ and Jacobi theta $\theta_3(z(\tau), t(\tau))$ functions,¹⁴ with modified arguments. The Dedekind eta is defined as an infinite product,

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

n=1¹⁴For the properties of this last special function, see, e.g. [49, 50]. In the notations of ref. [49], $\theta_3 \equiv \theta \begin{bmatrix} 0\\0 \end{bmatrix}$.

| Γ_N | $\Gamma_2 \simeq S_3$ | $\Gamma_3 \simeq A_4$ | $\Gamma_4 \simeq S_4$ | $\Gamma_5 \simeq A_5$ |
|---------------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Linear space dim. at weight k | k/2 + 1 | k+1 | 2k + 1 | 5k + 1 |
| Linear space dim. at weight 2 | 2 | 3 | 5 | 11 |
| Lowest weight irreps | 2 | 3 | $2,3^{\prime}$ | $3,3^{\prime},5$ |

Table 3. Dimensions of the linear spaces of modular forms at generic weight k and at the lowest weight (k = 2) [51], including the irrep breakdown at the lowest weight [21, 23, 30, 32], for the finite modular groups Γ_N with $N \leq 5$.

while the Jacobi θ_3 can be written as the series

$$\theta_3(z,\tau) = \sum_{n=-\infty}^{\infty} \tilde{q}^{n^2} e^{2\pi i n z}, \qquad \tilde{q} = e^{\pi i \tau}.$$
(C.2)

Below, for each $N \leq 5$, we reproduce explicit expressions for the lowest weight modular multiplets $Y_{\mathbf{r}}^{(N,k=2)}$ as vectors of the aforementioned log-derivatives. Note that these multiplets are given in the symmetric basis of appendix B.2. For these groups, the dimensions of linear spaces at different weights and the irreducible representations arising at lowest weight are summarised in table 3.

C.1.1 $\Gamma_2 \simeq S_3$

The lowest weight multiplet for Γ_2 was derived in ref. [23], and reads (up to normalisation):

$$Y_{\mathbf{2}}^{(2,2)}(\tau) = i \begin{pmatrix} Y^{(2)}(1,1,-2|\tau) \\ Y^{(2)}(\sqrt{3},-\sqrt{3},0|\tau) \end{pmatrix},$$
(C.3)

with

$$Y^{(2)}(a_1, a_2, a_3 | \tau) = \frac{d}{d\tau} \left[a_1 \log \eta \left(\frac{\tau}{2}\right) + a_2 \log \eta \left(\frac{\tau+1}{2}\right) + a_3 \log \eta \left(2\tau\right) \right].$$
(C.4)

C.1.2 $\Gamma_3 \simeq A_4$

The lowest weight multiplet for Γ_3 was derived in ref. [21], and reads (up to normalisation):

$$Y_{\mathbf{3}}^{(3,2)}(\tau) = i \begin{pmatrix} Y^{(3)}(1/2, 1/2, 1/2, -3/2|\tau) \\ -Y^{(3)}(1, \omega^2, \omega, 0|\tau) \\ -Y^{(3)}(1, \omega, \omega^2, 0|\tau) \end{pmatrix},$$
(C.5)

with $\omega = e^{2\pi i/3}$ and

$$Y^{(3)}(a_1, \dots, a_4 | \tau) = \frac{\mathrm{d}}{\mathrm{d}\tau} \left[a_1 \log \eta \left(\frac{\tau}{3}\right) + a_2 \log \eta \left(\frac{\tau+1}{3}\right) + a_3 \log \eta \left(\frac{\tau+2}{3}\right) + a_4 \log \eta \left(3\tau\right) \right].$$
(C.6)

C.1.3 $\Gamma_4 \simeq S_4$

The lowest weight multiplets for Γ_4 were derived in ref. [30], in a non-symmetric basis for the representation of group generators. In the symmetric basis we here consider, they read (up to normalisation):

$$Y_{\mathbf{2}}^{(4,2)}(\tau) = i \begin{pmatrix} Y^{(4)}(1,1,-1/2,-1/2,-1/2,-1/2|\tau) \\ Y^{(4)}(0,0,\sqrt{3}/2,-\sqrt{3}/2,\sqrt{3}/2,-\sqrt{3}/2|\tau) \end{pmatrix},$$
(C.7)

$$Y_{\mathbf{3'}}^{(4,2)}(\tau) = i \begin{pmatrix} Y^{(4)}(1, -1, 0, 0, 0, 0|\tau) \\ Y^{(4)}(0, 0, -1/\sqrt{2}, i/\sqrt{2}, 1/\sqrt{2}, -i/\sqrt{2}|\tau) \\ Y^{(4)}(0, 0, -1/\sqrt{2}, -i/\sqrt{2}, 1/\sqrt{2}, i/\sqrt{2}|\tau) \end{pmatrix},$$
(C.8)

with

$$Y^{(4)}(a_1, \dots, a_6 | \tau) = \frac{d}{d\tau} \left[a_1 \log \eta \left(\tau + \frac{1}{2} \right) + a_2 \log \eta \left(4\tau \right) + a_3 \log \eta \left(\frac{\tau}{4} \right) \right. \\ \left. + a_4 \log \eta \left(\frac{\tau + 1}{4} \right) + a_5 \log \eta \left(\frac{\tau + 2}{4} \right) + a_6 \log \eta \left(\frac{\tau + 3}{4} \right) \right].$$
(C.9)

C.1.4 $\Gamma_5 \simeq A_5$

The lowest weight multiplets for Γ_5 were derived in ref. [32], and read (up to normalisation):

$$\begin{split} Y_{\mathbf{5}}^{(5,2)}(\tau) &= i \begin{pmatrix} -\frac{1}{\sqrt{6}}Y^{(5)}\left(-5,1,1,1,1,1;-5,1,1,1,1,1|\tau\right) \\ Y^{(5)}(0,1,\zeta^{4},\zeta^{3},\zeta^{2},\zeta;0,1,\zeta^{4},\zeta^{3},\zeta^{2},\zeta|\tau) \\ Y^{(5)}(0,1,\zeta^{3},\zeta,\zeta^{4},\zeta^{2};0,1,\zeta^{3},\zeta,\zeta^{4},\zeta^{2}|\tau) \\ Y^{(5)}(0,1,\zeta^{2},\zeta^{4},\zeta,\zeta^{3};0,1,\zeta^{2},\zeta^{4},\zeta,\zeta^{3}|\tau) \\ Y^{(5)}(0,1,\zeta,\zeta^{2},\zeta^{3},\zeta^{4};0,1,\zeta,\zeta^{2},\zeta^{3},\zeta^{4}|\tau) \end{pmatrix}, \end{split}$$
(C.10)
$$\begin{aligned} Y_{\mathbf{3}}^{(5,2)}(\tau) &= i \begin{pmatrix} \frac{1}{\sqrt{2}}Y^{(5)}\left(-\sqrt{5},-1,-1,-1,-1,-1;\sqrt{5},1,1,1,1,1|\tau\right) \\ Y^{(5)}(0,1,\zeta^{4},\zeta^{3},\zeta^{2},\zeta;0,-1,-\zeta^{4},-\zeta^{3},-\zeta^{2},-\zeta|\tau) \\ Y^{(5)}(0,1,\zeta,\zeta^{2},\zeta^{3},\zeta^{4};0,-1,-\zeta,-\zeta^{2},-\zeta^{3},-\zeta^{4}|\tau) \end{pmatrix}, \end{aligned}$$
(C.11)
$$\begin{aligned} Y_{\mathbf{3'}}^{(5,2)}(\tau) &= i \begin{pmatrix} \frac{1}{\sqrt{2}}Y^{(5)}\left(\sqrt{5},-1,-1,-1,-1,-1,-1;-\sqrt{5},1,1,1,1,1|\tau\right) \\ Y^{(5)}(0,1,\zeta^{3},\zeta,\zeta^{4},\zeta^{2};0,-1,-\zeta^{3},-\zeta,-\zeta^{4},-\zeta^{2}|\tau) \\ Y^{(5)}(0,1,\zeta^{2},\zeta^{4},\zeta,\zeta^{3};0,-1,-\zeta^{2},-\zeta^{4},-\zeta,-\zeta^{3}|\tau) \end{pmatrix}, \end{aligned}$$
(C.12)

with $\zeta = e^{2\pi i/5}$ and

$$Y^{(5)}(c_{1,-1},\ldots,c_{1,4};c_{2,-1},\ldots,c_{2,4}|\tau) = \sum_{i,j} c_{i,j} \frac{\mathrm{d}}{\mathrm{d}\tau} \log \alpha_{i,j}(\tau), \qquad (C.13)$$

the corresponding seed functions being

$$\begin{aligned} \alpha_{1,-1}(\tau) &= \theta_3 \left(\frac{\tau+1}{2}, 5\tau \right), & \alpha_{2,-1}(\tau) = e^{2\pi i \tau/5} \theta_3 \left(\frac{3\tau+1}{2}, 5\tau \right), \\ \alpha_{1,0}(\tau) &= \theta_3 \left(\frac{\tau+9}{10}, \frac{\tau}{5} \right), & \alpha_{2,0}(\tau) = \theta_3 \left(\frac{\tau+7}{10}, \frac{\tau}{5} \right), \\ \alpha_{1,1}(\tau) &= \theta_3 \left(\frac{\tau+1}{10}, \frac{\tau+2}{5} \right), & \alpha_{2,1}(\tau) = \theta_3 \left(\frac{\tau+8}{10}, \frac{\tau+1}{5} \right), \\ \alpha_{1,2}(\tau) &= \theta_3 \left(\frac{\tau+1}{10}, \frac{\tau+2}{5} \right), & \alpha_{2,2}(\tau) = \theta_3 \left(\frac{\tau+9}{10}, \frac{\tau+2}{5} \right), \\ \alpha_{1,3}(\tau) &= \theta_3 \left(\frac{\tau+2}{10}, \frac{\tau+3}{5} \right), & \alpha_{2,3}(\tau) = \theta_3 \left(\frac{\tau+1}{10}, \frac{\tau+4}{5} \right), \\ \alpha_{1,4}(\tau) &= \theta_3 \left(\frac{\tau+3}{10}, \frac{\tau+4}{5} \right), & \alpha_{2,4}(\tau) = \theta_3 \left(\frac{\tau+1}{10}, \frac{\tau+4}{5} \right). \end{aligned}$$
(C.14)

C.2 Bases for spaces of lowest weight forms and their q-expansions

For each Γ_N , one can obtain q-expansions for a basis $b_i^{(N)}$ (the so-called Miller-like basis) of the space of lowest weight modular forms from the SageMath algebra system [52] (see, e.g., [32]). The dimensions of these linear spaces have been given in table 3. Below, for each $N \leq 5$, we present these expansions as well as the decompositions of the lowest weight multiplets of appendix C.1 (given in the symmetric basis of appendix B.2) in terms of the basis vectors $b_i^{(N)} \equiv b_i^{(N)}(\tau)$.

C.2.1 $\Gamma_2 \simeq S_3$

For Γ_2 , the Miller-like basis reads:

$$b_{1}^{(2)} = 1 + 24q_{2}^{2} + 24q_{2}^{4} + 96q_{2}^{6} + 24q_{2}^{8} + 144q_{2}^{10} + 96q_{2}^{12} + 192q_{2}^{14} + 24q_{2}^{16} + 312q_{2}^{18} + 144q_{2}^{20} + \dots,$$
(C.15)
$$b_{2}^{(2)} = q_{2} + 4q_{2}^{3} + 6q_{2}^{5} + 8q_{2}^{7} + 13q_{2}^{9} + 12q_{2}^{11} + 14q_{2}^{13} + 24q_{2}^{15} + 18q_{2}^{17} + 20q_{2}^{19} + \dots,$$

with $q_2 \equiv e^{2\pi i \tau/2} = e^{\pi i \tau}$. The lowest weight modular multiplet of Γ_2 can be written in terms of the above vectors, namely (see also [23]):

$$Y_{\mathbf{2}}^{(2,2)}(\tau) = 2\pi \begin{pmatrix} b_1^{(2)}(\tau)/8\\ \sqrt{3} b_2^{(2)}(\tau) \end{pmatrix}.$$
 (C.16)

In the present appendix, modular multiplets are properly normalised, guaranteeing $Y(-\tau^*) = Y^*(\tau)$.

C.2.2 $\Gamma_3 \simeq A_4$

For Γ_3 , the Miller-like basis reads:

$$\begin{split} b_1^{(3)} &= 1 + 12q_3^3 + 36q_3^6 + 12q_3^9 + 84q_3^{12} + 72q_3^{15} + 36q_3^{18} + 96q_3^{21} + 180q_3^{24} \\ &\quad + 12q_3^{27} + 216q_3^{30} + \dots, \end{split} \tag{C.17}$$

$$b_2^{(3)} &= q_3 + 7q_3^4 + 8q_3^7 + 18q_3^{10} + 14q_3^{13} + 31q_3^{16} + 20q_3^{19} + 36q_3^{22} + 31q_3^{25} + 56q_3^{28} + \dots, \\ b_3^{(3)} &= q_3^2 + 2q_3^5 + 5q_3^8 + 4q_3^{11} + 8q_3^{14} + 6q_3^{17} + 14q_3^{20} + 8q_3^{23} + 14q_3^{26} + 10q_3^{29} + \dots, \end{split}$$

with $q_3 \equiv e^{2\pi i \tau/3}$. The lowest weight modular multiplet of Γ_3 can be written in terms of the above vectors, namely (see also [21]):

$$Y_{\mathbf{3}}^{(3,2)}(\tau) = \frac{\pi}{3} \begin{pmatrix} b_1^{(3)}(\tau) \\ -6 \, b_2^{(3)}(\tau) \\ -18 \, b_3^{(3)}(\tau) \end{pmatrix}.$$
(C.18)

C.2.3 $\Gamma_4 \simeq S_4$

For Γ_4 , the Miller-like basis reads:

$$\begin{split} b_1^{(4)} &= 1 + 24q_4^8 + 24q_4^{16} + 96q_4^{24} + 24q_4^{32} + 144q_4^{40} + \dots, \\ b_2^{(4)} &= q_4 + 6q_5^5 + 13q_4^9 + 14q_4^{13} + 18q_4^{17} + 32q_4^{21} + 31q_4^{25} + 30q_4^{29} + 48q_4^{33} + 38q_4^{37} + \dots, \\ b_3^{(4)} &= q_4^2 + 4q_4^6 + 6q_4^{10} + 8q_4^{14} + 13q_4^{18} + 12q_4^{22} + 14q_4^{26} + 24q_4^{30} + 18q_4^{34} + 20q_4^{38} + \dots, \\ b_4^{(4)} &= q_4^3 + 2q_4^7 + 3q_4^{11} + 6q_4^{15} + 5q_4^{19} + 6q_4^{23} + 10q_4^{27} + 8q_4^{31} + 12q_4^{35} + 14q_4^{39} + \dots, \\ b_5^{(4)} &= q_4^4 + 4q_4^{12} + 6q_4^{20} + 8q_4^{28} + 13q_4^{36} + \dots, \end{split}$$
(C.19)

with $q_4 \equiv e^{2\pi i \tau/4} = e^{\pi i \tau/2}$. The lowest weight modular multiplets of Γ_4 can be written in terms of the above vectors, namely:

$$Y_{\mathbf{2}}^{(4,2)}(\tau) = -3\pi \begin{pmatrix} b_1^{(4)}(\tau)/8 + 3b_5^{(4)}(\tau) \\ -\sqrt{3}b_3^{(4)}(\tau) \end{pmatrix}, \qquad (C.20)$$

$$Y_{\mathbf{3'}}^{(4,2)}(\tau) = -\pi \begin{pmatrix} -b_1^{(4)}(\tau)/4 + 2 \, b_5^{(4)}(\tau) \\ \sqrt{2} \, b_2^{(4)}(\tau) \\ 4\sqrt{2} \, b_4^{(4)}(\tau) \end{pmatrix} .$$
(C.21)

C.2.4 $\Gamma_5 \simeq A_5$

For Γ_5 , the Miller-like basis reads:

$$\begin{split} b_1^{(5)} &= 1 + 60q_5^{15} - 120q_5^{20} + 240q_5^{25} - 300q_5^{30} + 300q_5^{35} - 180q_5^{45} + 240q_5^{50} + \dots , \\ b_2^{(5)} &= q_5 + 12q_5^{11} + 7q_5^{16} + 8q_5^{21} + 6q_5^{26} + 32q_5^{31} + 7q_5^{36} + 42q_5^{41} + 12q_5^{46} + \dots , \\ b_3^{(5)} &= q_5^2 + 12q_5^{12} - 2q_5^{17} + 12q_5^{22} + 8q_5^{27} + 21q_5^{32} - 6q_5^{37} + 48q_5^{42} - 8q_5^{47} + \dots , \\ b_4^{(5)} &= q_5^3 + 11q_5^{13} - 9q_5^{18} + 21q_5^{23} - q_5^{28} + 12q_5^{33} + 41q_5^{43} - 29q_5^{48} + \dots , \\ b_5^{(5)} &= q_5^4 + 9q_5^{14} - 12q_5^{19} + 29q_5^{24} - 18q_5^{29} + 17q_5^{34} + 8q_5^{39} + 12q_5^{44} - 16q_5^{49} + \dots , \\ b_6^{(5)} &= q_5^5 + 6q_5^{15} - 9q_5^{20} + 27q_5^{25} - 28q_5^{30} + 30q_5^{35} - 11q_5^{45} + 26q_5^{50} + \dots , \\ b_6^{(5)} &= q_5^6 + 2q_5^{16} + 2q_5^{21} + 3q_5^{26} + 7q_5^{36} + 5q_5^{46} + \dots , \\ b_7^{(5)} &= q_5^6 - q_5^{12} + 3q_5^{17} + 2q_5^{27} + 7q_5^{37} - 6q_5^{42} + 9q_5^{47} + \dots , \\ b_8^{(5)} &= q_5^7 - q_5^{12} + 3q_5^{17} + 2q_5^{27} + 7q_5^{37} - 6q_5^{42} + 9q_5^{43} + 16q_5^{48} + \dots , \\ b_{9}^{(5)} &= q_5^8 - 2q_5^{13} + 5q_5^{18} - 4q_5^{23} + 4q_5^{28} + 4q_5^{38} - 8q_5^{43} + 16q_5^{48} + \dots , \\ b_{10}^{(5)} &= q_5^9 - 3q_5^{14} + 8q_5^{19} - 11q_5^{24} + 12q_5^{29} - 5q_5^{34} + 13q_5^{49} + \dots , \\ b_{11}^{(5)} &= q_5^{10} - 4q_5^{15} + 12q_5^{20} - 22q_5^{25} + 30q_5^{30} - 24q_5^{35} + 5q_5^{40} + 18q_5^{45} - 21q_5^{50} + \dots , \end{split}$$

with $q_5 \equiv e^{2\pi i \tau/5}$. The lowest weight modular multiplets of Γ_5 can be written in terms of the above vectors, namely (see also [32]):

$$Y_{\mathbf{3}}^{(5,2)}(\tau) = -2\sqrt{5}\pi \begin{pmatrix} \left(b_{1}^{(5)}(\tau) - 30 \, b_{6}^{(5)}(\tau) - 20 \, b_{11}^{(5)}(\tau)\right) / (5\sqrt{2}) \\ b_{2}^{(5)}(\tau) + 2 \, b_{7}^{(5)}(\tau) \\ 3 \, b_{5}^{(5)}(\tau) + 7 \, b_{10}^{(5)}(\tau) \end{pmatrix}, \qquad (C.23)$$

$$Y_{\mathbf{3}'}^{(5,2)}(\tau) = -2\sqrt{5}\pi \begin{pmatrix} -\left(b_1^{(5)}(\tau) + 20 \, b_6^{(5)}(\tau) + 30 \, b_{11}^{(5)}(\tau)\right) / (5\sqrt{2}) \\ b_3^{(5)}(\tau) + 6 \, b_8^{(5)}(\tau) \\ 2 \, b_4^{(5)}(\tau) + 5 \, b_9^{(5)}(\tau) \end{pmatrix}, \quad (C.24)$$

$$Y_{\mathbf{5}}^{(5,2)}(\tau) = 2\pi \begin{pmatrix} -\left(b_{1}^{(5)}(\tau) + 6\,b_{6}^{(5)}(\tau) + 18\,b_{11}^{(5)}(\tau)\right)/\sqrt{6} \\ b_{2}^{(5)}(\tau) + 12\,b_{7}^{(5)}(\tau) \\ 3\,b_{3}^{(5)}(\tau) + 8\,b_{8}^{(5)}(\tau) \\ 4\,b_{4}^{(5)}(\tau) + 15\,b_{9}^{(5)}(\tau) \\ 7\,b_{5}^{(5)}(\tau) + 13\,b_{10}^{(5)}(\tau) \end{pmatrix} \right).$$
(C.25)

C.3 Higher weight multiplets for $\Gamma_4 \simeq S_4$ in the symmetric basis

Multiplets of higher weight $Y_{\mathbf{r},\mu}^{(N,k>2)}$, with the index μ labelling linearly independent multiplets, may be obtained from those of lower weight via tensor products. For Γ_3 , multiplets of weight up to 6 are found in ref. [21], while for Γ_4 and Γ_5 , multiplets of weight up to 10 are given in refs. [31] and [32], respectively.

Since in [31] the considered basis for Γ_4 is not a symmetric one, we here present explicit expressions for higher weight multiplets in the symmetric basis of appendix B.2. Making use of the shorthands $Y_2^{(4,2)} = (Y_1, Y_2)^T$ and $Y_{3'}^{(4,2)} = (Y_3, Y_4, Y_5)^T$, one has at weight 4,

$$Y_{\mathbf{1}}^{(4,4)} = Y_{\mathbf{1}}^{2} + Y_{\mathbf{2}}^{2}, \qquad Y_{\mathbf{2}}^{(4,4)} = \begin{pmatrix} Y_{\mathbf{2}}^{2} - Y_{\mathbf{1}}^{2} \\ 2Y_{\mathbf{1}}Y_{\mathbf{2}} \end{pmatrix},$$
$$Y_{\mathbf{3}}^{(4,4)} = \begin{pmatrix} -2Y_{2}Y_{3} \\ \sqrt{3}Y_{1}Y_{5} + Y_{2}Y_{4} \\ \sqrt{3}Y_{1}Y_{4} + Y_{2}Y_{5} \end{pmatrix}, \qquad Y_{\mathbf{3'}}^{(4,4)} = \begin{pmatrix} 2Y_{1}Y_{3} \\ \sqrt{3}Y_{2}Y_{5} - Y_{1}Y_{4} \\ \sqrt{3}Y_{2}Y_{4} - Y_{1}Y_{5} \end{pmatrix}, \qquad (C.26)$$

at weight 6,

$$Y_{\mathbf{1}}^{(4,6)} = Y_{1} \left(3Y_{2}^{2} - Y_{1}^{2} \right), \qquad Y_{\mathbf{1}'}^{(4,6)} = Y_{2} \left(3Y_{1}^{2} - Y_{2}^{2} \right),$$

$$Y_{\mathbf{2}}^{(4,6)} = \left(Y_{1}^{2} + Y_{2}^{2} \right) \begin{pmatrix} Y_{1} \\ Y_{2} \end{pmatrix}, \qquad Y_{\mathbf{3}}^{(4,6)} = \begin{pmatrix} Y_{1} \left(Y_{4}^{2} - Y_{5}^{2} \right) \\ Y_{3} \left(Y_{1}Y_{5} + \sqrt{3}Y_{2}Y_{4} \right) \\ -Y_{3} \left(Y_{1}Y_{4} + \sqrt{3}Y_{2}Y_{5} \right) \end{pmatrix},$$

$$Y_{\mathbf{3}',1}^{(4,6)} = \left(Y_{1}^{2} + Y_{2}^{2} \right) \begin{pmatrix} Y_{3} \\ Y_{4} \\ Y_{5} \end{pmatrix}, \qquad Y_{\mathbf{3}',2}^{(4,6)} = \begin{pmatrix} Y_{2} \left(Y_{5}^{2} - Y_{4}^{2} \right) \\ -Y_{3} \left(Y_{2}Y_{5} - \sqrt{3}Y_{1}Y_{4} \right) \\ Y_{3} \left(Y_{2}Y_{4} - \sqrt{3}Y_{1}Y_{5} \right) \end{pmatrix}, \qquad (C.27)$$

at weight 8,

$$\begin{split} Y_{1}^{(4,8)} &= \left(Y_{1}^{2} + Y_{2}^{2}\right)^{2}, \\ Y_{2,1}^{(4,8)} &= \left(Y_{1}^{2} + Y_{2}^{2}\right) \begin{pmatrix} Y_{2}^{2} - Y_{1}^{2} \\ 2Y_{1}Y_{2} \end{pmatrix}, \\ Y_{3,1}^{(4,8)} &= \left(Y_{1}^{2} + Y_{2}^{2}\right) \begin{pmatrix} -2Y_{2}Y_{3} \\ Y_{2}Y_{4} + \sqrt{3}Y_{1}Y_{5} \\ Y_{2}Y_{5} + \sqrt{3}Y_{1}Y_{4} \end{pmatrix}, \\ Y_{3',1}^{(4,8)} &= \left(Y_{1}^{2} + Y_{2}^{2}\right) \begin{pmatrix} -2Y_{1}Y_{3} \\ Y_{2}Y_{5} + \sqrt{3}Y_{1}Y_{4} \end{pmatrix}, \\ Y_{3',1}^{(4,8)} &= \left(Y_{1}^{2} + Y_{2}^{2}\right) \begin{pmatrix} -2Y_{1}Y_{3} \\ Y_{1}Y_{4} - \sqrt{3}Y_{2}Y_{5} \\ Y_{1}Y_{5} - \sqrt{3}Y_{2}Y_{4} \end{pmatrix}, \\ Y_{3',2}^{(4,8)} &= Y_{1} \left(Y_{1}^{2} - 3Y_{2}^{2}\right) \begin{pmatrix} Y_{3} \\ Y_{4} \\ Y_{5} \end{pmatrix}, \\ (C.28) \end{split}$$

and at weight 10,

$$\begin{split} Y_{1}^{(4,10)} &= Y_{1} \left(Y_{1}^{2} - 3 Y_{2}^{2} \right) \left(Y_{1}^{2} + Y_{2}^{2} \right) , \qquad Y_{1'}^{(4,10)} = Y_{2} \left(Y_{2}^{2} - 3 Y_{1}^{2} \right) \left(Y_{1}^{2} + Y_{2}^{2} \right) , \\ Y_{2,1}^{(4,10)} &= \left(Y_{1}^{2} + Y_{2}^{2} \right)^{2} \begin{pmatrix} Y_{1} \\ Y_{2} \end{pmatrix} , \qquad Y_{2,2}^{(4,10)} = \left(Y_{1}^{2} - 3 Y_{2}^{2} \right) \begin{pmatrix} Y_{1}^{3} - Y_{1}Y_{2}^{2} \\ -2 Y_{1}^{2}Y_{2} \end{pmatrix} , \\ Y_{3,1}^{(4,10)} &= Y_{1} \left(Y_{1}^{2} - 3 Y_{2}^{2} \right) \begin{pmatrix} -2 Y_{2}Y_{3} \\ Y_{2}Y_{4} + \sqrt{3} Y_{1}Y_{5} \\ Y_{2}Y_{5} + \sqrt{3} Y_{1}Y_{4} \end{pmatrix} , \qquad Y_{3,2}^{(4,10)} = Y_{2} \left(Y_{2}^{2} - 3 Y_{1}^{2} \right) \begin{pmatrix} -2 Y_{1}Y_{3} \\ Y_{1}Y_{4} - \sqrt{3} Y_{2}Y_{5} \\ Y_{1}Y_{5} - \sqrt{3} Y_{2}Y_{4} \end{pmatrix} , \\ Y_{3',1}^{(4,10)} &= Y_{1} \left(Y_{1}^{2} - 3 Y_{2}^{2} \right) \begin{pmatrix} -2 Y_{1}Y_{3} \\ Y_{1}Y_{4} - \sqrt{3} Y_{2}Y_{5} \\ Y_{1}Y_{5} - \sqrt{3} Y_{2}Y_{4} \end{pmatrix} , \qquad Y_{3',2}^{(4,10)} = Y_{2} \left(Y_{2}^{2} - 3 Y_{1}^{2} \right) \begin{pmatrix} -2 Y_{2}Y_{3} \\ Y_{2}Y_{4} + \sqrt{3} Y_{1}Y_{5} \\ Y_{2}Y_{5} + \sqrt{3} Y_{1}Y_{4} \end{pmatrix} , \\ Y_{3',3}^{(4,10)} &= \left(Y_{1}^{2} + Y_{2}^{2} \right)^{2} \begin{pmatrix} Y_{3} \\ Y_{4} \\ Y_{5} \end{pmatrix} . \qquad (C.29)$$

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