

# Spontaneous CP violation by modulus $\tau$ in $A_4$ model of lepton flavors

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**ABSTRACT:** We discuss the modular  $A_4$  invariant model of leptons combining with the generalized CP symmetry. In our model, both CP and modular symmetries are broken spontaneously by the vacuum expectation value of the modulus  $\tau$ . The source of the CP violation is a non-trivial value of  $\text{Re}[\tau]$  while other parameters of the model are real. The allowed region of  $\tau$  is in very narrow one close to the fixed point  $\tau = i$  for both normal hierarchy (NH) and inverted ones (IH) of neutrino masses. The CP violating Dirac phase  $\delta_{\text{CP}}$  is predicted clearly in  $[98^\circ, 110^\circ]$  and  $[250^\circ, 262^\circ]$  for NH at  $3\sigma$  confidence level. On the other hand,  $\delta_{\text{CP}}$  is in  $[95^\circ, 100^\circ]$  and  $[260^\circ, 265^\circ]$  for IH at  $5\sigma$  confidence level. The predicted  $\sum m_i$  is in  $[82, 102]$  meV for NH and  $\sum m_i = [134, 180]$  meV for IH. The effective mass  $\langle m_{ee} \rangle$  for the  $0\nu\beta\beta$  decay is predicted in  $[12.5, 20.5]$  meV and  $[54, 67]$  meV for NH and IH, respectively.

**KEYWORDS:** CP violation, Discrete Symmetries, Neutrino Physics

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## 1 Introduction

The non-Abelian discrete symmetries are attractive ones to understand flavors of quarks and leptons. The  $S_3$  flavor symmetry was a pioneer for the quark flavor mixing [1, 2]. It was also discussed to understand the large mixing angle [3] in the oscillation of atmospheric neutrinos [4]. For the last twenty years, the non-Abelian discrete symmetries of flavors have been developed, that is motivated by the precise observation of flavor mixing angles of leptons [5–14]. Among them, the  $A_4$  flavor model is an attractive one because the  $A_4$  group is the minimal one including a triplet irreducible representation, which allows for a natural explanation of the existence of three families of quarks and leptons [15–21]. However, it is difficult to obtain clear predictions of the  $A_4$  flavor symmetry because of a lot of free parameters associated with scalar flavon fields.

Recently, a new approach to the lepton flavor problem has been put forward based on the invariance under the modular transformation [22], where the model of the finite modular

group  $\Gamma_3 \simeq A_4$  has been presented. In this approach, fermion matrices are written in terms of modular forms which are holomorphic functions of the modulus  $\tau$ . This work inspired further studies of the modular invariance approach to the lepton flavor problem.

The finite groups  $S_3$ ,  $A_4$ ,  $S_4$ , and  $A_5$  are realized in modular groups [23]. Modular invariant flavor models have been also proposed on the  $\Gamma_2 \simeq S_3$  [24],  $\Gamma_4 \simeq S_4$  [25] and  $\Gamma_5 \simeq A_5$  [26]. Phenomenological discussions of the neutrino flavor mixing have been done based on  $A_4$  [27–29],  $S_4$  [30–32] and  $A_5$  [33]. A clear prediction of the neutrino mixing angles and the CP violating phase was given in the simple lepton mass matrices with the  $A_4$  modular symmetry [28]. On the other hand, the Double Covering groups  $T'$  [34, 35] and  $S'_4$  [36, 37] were realized in the modular symmetry. Furthermore, modular forms for  $\Delta(96)$  and  $\Delta(384)$  were constructed [38], and the extension of the traditional flavor group was discussed with modular symmetries [39]. The level 7 finite modular group  $\Gamma_7 \simeq \text{PSL}(2, Z_7)$  was also presented for the lepton mixing [40]. Based on those works, phenomenological studies have been developed in many works [41–80] while theoretical investigations have been also proceeded [81–86].

In order to test the modular symmetry of flavors, the prediction of the CP violating Dirac phase is important. The CP transformation is non-trivial if the non-Abelian discrete flavor symmetry is set in the Yukawa sector of a Lagrangian. Then, we should discuss so called the generalized CP symmetry in the flavor space [87–91]. It can predict the CP violating phase [92]. The modular invariance has been also studied combining with the generalized CP symmetry in flavor theories [93, 94]. It provides a powerful framework to predict CP violating phases of quarks and leptons.

In our work, we present the modular  $A_4$  invariant model with the generalized CP symmetry. Both CP and modular symmetries are broken spontaneously by the vacuum expectation value (VEV) of the modulus  $\tau$ . We discuss the phenomenological implication of this model, that is the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) mixing angles [95, 96] and the CP violating Dirac phase of leptons, which is expected to be observed at T2K and  $\text{NO}\nu A$  experiments [97, 98].

The paper is organized as follows. In section 2, we give a brief review on the generalized CP transformation in the modular symmetry. In section 3, we present the CP invariant lepton mass matrix in the  $A_4$  modular symmetry. In section 4, we show the phenomenological implication of our model. section 5 is devoted to the summary. In appendix A, we present the tensor product of the  $A_4$  group. In appendix B, we show the modular forms for weight 2 and 4. In appendix C, we show how to determine the coupling coefficients of the charged lepton sector. In appendix D, we present how to obtain the Dirac  $CP$  phase, the Majorana phases and the effective mass of the  $0\nu\beta\beta$  decay.

## 2 Generalized CP transformation in modular symmetry

### 2.1 Generalized CP symmetry

Let us start with discussing the generalised  $CP$  symmetry [92, 99]. The CP transformation is non-trivial if the non-Abelian discrete flavor symmetry  $G$  is set in the Yukawa sector of a Lagrangian. Let us consider the chiral superfields. The CP is a discrete symmetry

which involves both Hermitian conjugation of a chiral superfield  $\psi(x)$  and inversion of spatial coordinates,

$$\psi(x) \rightarrow \mathbf{X}_{\mathbf{r}} \bar{\psi}(x_P), \quad (2.1)$$

where  $x_P = (t, -\mathbf{x})$  and  $\mathbf{X}_{\mathbf{r}}$  is a unitary transformations of  $\psi(x)$  in the irreducible representation  $\mathbf{r}$  of the discrete flavor symmetry  $G$ . If  $\mathbf{X}_{\mathbf{r}}$  is the unit matrix, the  $CP$  transformation is the trivial one. This is the case for the continuous flavor symmetry [99]. However, in the framework of the non-Abelian discrete family symmetry, non-trivial choices of  $\mathbf{X}_{\mathbf{r}}$  are possible. The unbroken  $CP$  transformations of  $\mathbf{X}_{\mathbf{r}}$  form the group  $H_{CP}$ . Then,  $\mathbf{X}_{\mathbf{r}}$  must be consistent with the flavor symmetry transformation,

$$\psi(x) \rightarrow \rho_{\mathbf{r}}(g)\psi(x), \quad g \in G, \quad (2.2)$$

where  $\rho_{\mathbf{r}}(g)$  is the representation matrix for  $g$  in the irreducible representation  $\mathbf{r}$ .

The consistent condition is obtained as follows. At first, perform a  $CP$  transformation  $\psi(x) \rightarrow \mathbf{X}_{\mathbf{r}} \bar{\psi}(x_P)$ , then apply a flavor symmetry transformation,  $\bar{\psi}(x_P) \rightarrow \rho_{\mathbf{r}}^*(g)\bar{\psi}(x_P)$ , and finally perform an inverse  $CP$  transformation. The whole transformation is written as  $\psi(x) \rightarrow \mathbf{X}_{\mathbf{r}} \rho_{\mathbf{r}}^*(g) \mathbf{X}_{\mathbf{r}}^{-1} \psi(x)$ , which must be equivalent to some flavor symmetry  $\psi(x) \rightarrow \rho_{\mathbf{r}}(g')\psi(x)$ . Thus, one obtains [100]

$$\mathbf{X}_{\mathbf{r}} \rho_{\mathbf{r}}^*(g) \mathbf{X}_{\mathbf{r}}^{-1} = \rho_{\mathbf{r}}(g'), \quad g, g' \in G. \quad (2.3)$$

This equation defines the consistency condition, which has to be respected for consistent implementation of a generalized  $CP$  symmetry along with a flavor symmetry [101, 102]. This chain  $CP \rightarrow g \rightarrow CP^{-1}$  maps the group element  $g$  onto  $g'$  and preserves the flavor symmetry group structure. That is a homomorphism  $v(g) = g'$  of  $G$ . Assuming the presence of faithful representations  $\mathbf{r}$ , eq. (2.3) defines a unique mapping of  $G$  to itself. In this case,  $v(g)$  is an automorphism of  $G$  [101].

It has been also shown that the full symmetry group is isomorphic to a semi-direct product of  $G$  and  $H_{CP}$ , that is  $G \rtimes H_{CP}$ , where  $H_{CP} \simeq \mathbb{Z}_2^{CP}$ , is the group generated by the generalised  $CP$  transformation under the assumption of  $\mathbf{X}_{\mathbf{r}}$  being a symmetric matrix [102].

## 2.2 Modular symmetry

The modular group  $\bar{\Gamma}$  is the group of linear fractional transformations  $\gamma$  acting on the modulus  $\tau$ , belonging to the upper-half complex plane as:

$$\tau \longrightarrow \gamma\tau = \frac{a\tau + b}{c\tau + d}, \quad \text{where } a, b, c, d \in \mathbb{Z} \text{ and } ad - bc = 1, \quad \text{Im}[\tau] > 0, \quad (2.4)$$

which is isomorphic to  $\text{PSL}(2, \mathbb{Z}) = \text{SL}(2, \mathbb{Z}) / \{\mathbf{I}, -\mathbf{I}\}$  transformation. This modular transformation is generated by  $S$  and  $T$ ,

$$S : \tau \longrightarrow -\frac{1}{\tau}, \quad T : \tau \longrightarrow \tau + 1, \quad (2.5)$$

which satisfy the following algebraic relations,

$$S^2 = \mathbf{1}, \quad (ST)^3 = \mathbf{1}. \quad (2.6)$$

We introduce the series of groups  $\Gamma(N)$ , called principal congruence subgroups, where  $N$  is the level  $1, 2, 3, \dots$ . These groups are defined by

$$\Gamma(N) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}(2, \mathbb{Z}), \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \pmod{N} \right\}. \quad (2.7)$$

For  $N = 2$ , we define  $\bar{\Gamma}(2) \equiv \Gamma(2)/\{\mathbb{I}, -\mathbb{I}\}$ . Since the element  $-\mathbb{I}$  does not belong to  $\Gamma(N)$  for  $N > 2$ , we have  $\bar{\Gamma}(N) = \Gamma(N)$ . The quotient groups defined as  $\Gamma_N \equiv \bar{\Gamma}/\bar{\Gamma}(N)$  are finite modular groups. In these finite groups  $\Gamma_N$ ,  $T^N = \mathbb{1}$  is imposed. The groups  $\Gamma_N$  with  $N = 2, 3, 4, 5$  are isomorphic to  $S_3, A_4, S_4$  and  $A_5$ , respectively [23].

Modular forms  $f_i(\tau)$  of weight  $k$  are the holomorphic functions of  $\tau$  and transform as

$$f_i(\tau) \longrightarrow (c\tau + d)^k \rho(\gamma)_{ij} f_j(\tau), \quad \gamma \in G, \quad (2.8)$$

under the modular symmetry, where  $\rho(\gamma)_{ij}$  is a unitary matrix under  $\Gamma_N$ .

Superstring theory on the torus  $T^2$  or orbifold  $T^2/Z_N$  has the modular symmetry [103–109]. Its low energy effective field theory is described in terms of supergravity theory, and string-derived supergravity theory has also the modular symmetry. Under the modular transformation of eq. (2.4), chiral superfields  $\psi_i$  ( $i$  denotes flavors) transform as [110],

$$\psi_i \longrightarrow (c\tau + d)^{-k_I} \rho(\gamma)_{ij} \psi_j. \quad (2.9)$$

We study global supersymmetric models, e.g., minimal supersymmetric extensions of the Standard Model (MSSM). The superpotential which is built from matter fields and modular forms is assumed to be modular invariant, i.e., to have a vanishing modular weight. For given modular forms this can be achieved by assigning appropriate weights to the matter superfields.

The kinetic terms are derived from a Kähler potential. The Kähler potential of chiral matter fields  $\psi_i$  with the modular weight  $-k$  is given simply by

$$K^{\text{matter}} = \frac{1}{[i(\bar{\tau} - \tau)]^k} \sum_i |\psi_i|^2, \quad (2.10)$$

where the superfield and its scalar component are denoted by the same letter, and  $\bar{\tau} = \tau^*$  after taking VEV of  $\tau$ . Therefore, the canonical form of the kinetic terms is obtained by changing the normalization of parameters [28]. The general Kähler potential consistent with the modular symmetry possibly contains additional terms [111]. However, we consider only the simplest form of the Kähler potential.

For  $\Gamma_3 \simeq A_4$ , the dimension of the linear space  $\mathcal{M}_k(\Gamma(3))$  of modular forms of weight  $k$  is  $k + 1$  [112–114], i.e., there are three linearly independent modular forms of the lowest non-trivial weight 2, which form a triplet of the  $A_4$  group,  $\mathbf{Y}_3^{(2)}(\tau) = (Y_1(\tau), Y_2(\tau), Y_3(\tau))^T$ . As shown in appendix A, these modular forms have been explicitly obtained [22] in the symmetric base of the  $A_4$  generators  $S$  and  $T$  for the triplet representation:

$$S = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \quad (2.11)$$

where  $\omega = \exp(i\frac{2}{3}\pi)$ .

### 2.3 CP transformation of the modulus $\tau$

The CP transformation in the modular symmetry was given by using the generalized CP symmetry [93]. We summarize the discussion in ref. [93] briefly. Consider the CP and modular transformation  $\gamma$  of the chiral superfield  $\psi(x)$  assigned to an irreducible unitary representation  $\mathbf{r}$  of  $\Gamma_N$ . The chain  $CP \rightarrow \gamma \rightarrow CP^{-1} = \gamma' \in \bar{\Gamma}$  is expressed as:

$$\begin{aligned} \psi(x) &\xrightarrow{CP} \mathbf{X}_{\mathbf{r}} \bar{\psi}(x_P) \xrightarrow{\gamma} (c\tau^* + d)^{-k} \mathbf{X}_{\mathbf{r}} \rho_{\mathbf{r}}^*(\gamma) \bar{\psi}(x_P) \\ &\xrightarrow{CP^{-1}} (c\tau_{CP^{-1}}^* + d)^{-k} \mathbf{X}_{\mathbf{r}} \rho_{\mathbf{r}}^*(\gamma) \mathbf{X}_{\mathbf{r}}^{-1} \psi(x), \end{aligned} \quad (2.12)$$

where  $\tau_{CP^{-1}}$  is the operation of  $CP^{-1}$  on  $\tau$ . The result of this chain transformation should be equivalent to a modular transformation  $\gamma'$  which maps  $\psi(x)$  to  $(c'\tau + d')^{-k} \rho_{\mathbf{r}}(\gamma') \psi(x)$ . Therefore, one obtains

$$\mathbf{X}_{\mathbf{r}} \rho_{\mathbf{r}}^*(\gamma) \mathbf{X}_{\mathbf{r}}^{-1} = \left( \frac{c'\tau + d'}{c\tau_{CP^{-1}}^* + d} \right)^{-k} \rho_{\mathbf{r}}(\gamma'). \quad (2.13)$$

Since  $\mathbf{X}_{\mathbf{r}}$ ,  $\rho_{\mathbf{r}}$  and  $\rho_{\mathbf{r}'}$  are independent of  $\tau$ , the overall coefficient on the right-hand side of eq. (2.13) has to be a constant (complex) for non-zero weight  $k$ :

$$\frac{c'\tau + d'}{c\tau_{CP^{-1}}^* + d} = \frac{1}{\lambda^*}, \quad (2.14)$$

where  $|\lambda| = 1$  due to the unitarity of  $\rho_{\mathbf{r}}$  and  $\rho_{\mathbf{r}'}$ . The values of  $\lambda$ ,  $c'$  and  $d'$  depend on  $\gamma$ .

Taking  $\gamma = S$  ( $c = 1, d = 0$ ), and denoting  $c'(S) = C$ ,  $d'(S) = D$  while keeping  $\lambda(S) = \lambda$ , we find  $\tau = (\lambda\tau_{CP^{-1}}^* - D)/C$  from eq. (2.14), and consequently,

$$\tau \xrightarrow{CP^{-1}} \tau_{CP^{-1}} = \lambda(C\tau^* + D), \quad \tau \xrightarrow{CP} \tau_{CP} = \frac{1}{C}(\lambda\tau^* - D). \quad (2.15)$$

Let us act with chain  $CP \rightarrow T \rightarrow CP^{-1}$  on the modular  $\tau$  itself:

$$\tau \xrightarrow{CP} \tau_{CP} = \frac{1}{C}(\lambda\tau^* - D) \xrightarrow{T} \frac{1}{C}(\lambda(\tau^* + 1) - D) \xrightarrow{CP^{-1}} \tau + \frac{\lambda}{C}. \quad (2.16)$$

The resulting transformation has to be a modular transformation, therefore  $\lambda/C$  is an integer. Since  $|\lambda| = 1$ , we find  $|C| = 1$  and  $\lambda = \pm 1$ . After choosing the sign of  $C$  as  $C = \mp 1$  so that  $\text{Im}[\tau_{CP}] > 0$ , the CP transformation of eq. (2.15) turns to

$$\tau \xrightarrow{CP} n - \tau^*, \quad (2.17)$$

where  $n$  is an integer. The chain  $CP \rightarrow S \rightarrow CP^{-1} = \gamma'(S)$  imposes no further restrictions on  $\tau_{CP}$ . It is always possible to redefine the CP transformation in such a way that  $n = 0$  by using the freedom of  $T$  transformation. Therefore, we define that the modulus  $\tau$  transforms under CP as

$$\tau \xrightarrow{CP} -\tau^*, \quad (2.18)$$

without loss of generality.

The same transformation of  $\tau$  was also derived from the higher dimensional theories [94]. The four-dimensional CP symmetry can be embedded into  $(4 + d)$  dimensions as higher dimensional proper Lorentz symmetry with positive determinant. That is, one can combine the four-dimensional CP transformation and  $d$ -dimensional transformation with negative determinant so as to obtain  $(4 + d)$  dimensional proper Lorentz transformation. For example in six-dimensional theory, we denote the two extra coordinates by a complex coordinate  $z$ . The four-dimensional CP symmetry with  $z \rightarrow z^*$  or  $z \rightarrow -z^*$  is a six-dimensional proper Lorentz symmetry. Note that  $z = x + \tau y$ , where  $x$  and  $y$  are real coordinates. The latter transformation  $z \rightarrow -z^*$  maps the upper half plane  $\text{Im}[\tau] > 0$  to the same half plane. Hence, we consider the transformation  $z \rightarrow -z^*$  ( $\tau \rightarrow -\tau^*$ ) as the CP symmetry.

## 2.4 CP transformation of modular multiplets

Chiral superfields and modular forms transform in eqs. (2.8) and (2.9), respectively, under a modular transformation. Chiral superfields also transform in eq. (2.1) under the CP transformation. The CP transformation of modular forms were given in ref. [93] as follows. Define a modular multiplet of the irreducible representation  $\mathbf{r}$  of  $\Gamma_N$  with weight  $k$  as  $\mathbf{Y}_{\mathbf{r}}^{(k)}(\tau)$ , which is transformed as:

$$\mathbf{Y}_{\mathbf{r}}^{(k)}(\tau) \xrightarrow{\text{CP}} \mathbf{Y}_{\mathbf{r}}^{(k)}(-\tau^*), \quad (2.19)$$

under the CP transformation. The complex conjugated CP transformed modular forms  $\mathbf{Y}_{\mathbf{r}}^{(k)*}(-\tau^*)$  transform almost like the original multiplets  $\mathbf{Y}_{\mathbf{r}}^{(k)}(\tau)$  under a modular transformation, namely:

$$\mathbf{Y}_{\mathbf{r}}^{(k)*}(-\tau^*) \xrightarrow{\gamma} \mathbf{Y}_{\mathbf{r}}^{(k)*}(-(\gamma\tau)^*) = (c\tau + d)^k \rho_{\mathbf{r}}^*(u(\gamma)) \mathbf{Y}_{\mathbf{r}}^{(k)*}(-\tau^*), \quad (2.20)$$

where  $u(\gamma) \equiv CP\gamma CP^{-1}$ . Using the consistency condition of eq. (2.3), we obtain

$$\mathbf{X}_{\mathbf{r}}^{\mathbf{T}} \mathbf{Y}_{\mathbf{r}}^{(k)*}(-\tau^*) \xrightarrow{\gamma} (c\tau + d)^k \rho_{\mathbf{r}}(\gamma) \mathbf{X}_{\mathbf{r}}^{\mathbf{T}} \mathbf{Y}_{\mathbf{r}}^{(k)*}(-\tau^*). \quad (2.21)$$

Therefore, if there exist a unique modular multiplet at a level  $N$ , weight  $k$  and representation  $\mathbf{r}$ , which is satisfied for  $N = 2-5$  with weight 2, we can express the modular form  $\mathbf{Y}_{\mathbf{r}}^{(k)}(\tau)$  as:

$$\mathbf{Y}_{\mathbf{r}}^{(k)}(\tau) = \kappa \mathbf{X}_{\mathbf{r}}^{\mathbf{T}} \mathbf{Y}_{\mathbf{r}}^{(k)*}(-\tau^*), \quad (2.22)$$

where  $\kappa$  is a proportional coefficient. Since  $\mathbf{Y}_{\mathbf{r}}^{(k)}(-(-\tau^*)^*) = \mathbf{Y}_{\mathbf{r}}^{(k)}(\tau)$ , eq. (2.22) gives  $\mathbf{X}_{\mathbf{r}}^* \mathbf{X}_{\mathbf{r}} = |\kappa|^2 \mathbb{1}_{\mathbf{r}}$ . Therefore, the matrix  $\mathbf{X}_{\mathbf{r}}$  is symmetric one, and  $\kappa = e^{i\phi}$  is a phase, which can be absorbed in the normalization of modular forms. In conclusion, the CP transformation of modular forms is given as:

$$\mathbf{Y}_{\mathbf{r}}^{(k)}(\tau) \xrightarrow{\text{CP}} \mathbf{Y}_{\mathbf{r}}^{(k)}(-\tau^*) = \mathbf{X}_{\mathbf{r}} \mathbf{Y}_{\mathbf{r}}^{(k)*}(\tau). \quad (2.23)$$

It is also emphasized that  $\mathbf{X}_{\mathbf{r}} = \mathbb{1}_{\mathbf{r}}$  satisfies the consistency condition eq. (2.3) in a basis that generators of  $S$  and  $T$  of  $\Gamma_N$  are represented by symmetric matrices because of  $\rho_{\mathbf{r}}^*(S) = \rho_{\mathbf{r}}^{\dagger}(S) = \rho_{\mathbf{r}}(S^{-1}) = \rho_{\mathbf{r}}(S)$  and  $\rho_{\mathbf{r}}^*(T) = \rho_{\mathbf{r}}^{\dagger}(T) = \rho_{\mathbf{r}}(T^{-1})$ .

	$L$	$(e^c, \mu^c, \tau^c)$	$H_u$	$H_d$	$\mathbf{Y}_r^{(2)}, \mathbf{Y}_r^{(4)}$
SU(2)	<b>2</b>	<b>1</b>	<b>2</b>	<b>2</b>	<b>1</b>
$A_4$	<b>3</b>	$(\mathbf{1}, \mathbf{1}'', \mathbf{1}')$	<b>1</b>	<b>1</b>	<b>3, {3, 1, 1'}</b>
$k$	-2	$(0, 0, 0)$	0	0	2, 4

**Table 1.** Representations and weights  $k$  for MSSM fields and modular forms of weight 2 and 4.

The CP transformations of chiral superfields and modular multiplets are summarized as follows:

$$\tau \xrightarrow{\text{CP}} -\tau^*, \quad \psi(x) \xrightarrow{\text{CP}} X_r \bar{\psi}(x_P), \quad \mathbf{Y}_r^{(k)}(\tau) \xrightarrow{\text{CP}} \mathbf{Y}_r^{(k)}(-\tau^*) = \mathbf{X}_r \mathbf{Y}_r^{(k)*}(\tau), \quad (2.24)$$

where  $\mathbf{X}_r = \mathbb{1}_r$  can be taken in the base of symmetric generators of  $S$  and  $T$ . We use this CP transformation of modular forms to construct the CP invariant mass matrices in the next section.

### 3 CP invariant mass matrix in $A_4$ modular symmetry

Let us discuss the CP invariant lepton mass matrix in the framework of the  $A_4$  modular symmetry. We assign the  $A_4$  representation and weight for superfields of leptons in table 1, where the three left-handed lepton doublets compose a  $A_4$  triplet  $L$ , and the right-handed charged leptons  $e^c$ ,  $\mu^c$  and  $\tau^c$  are  $A_4$  singlets. The weights of the superfields of left-handed leptons and right-handed charged leptons are  $-2$  and  $0$ , respectively. Then, the simple lepton mass matrices for charged leptons and neutrinos are obtained [75].

The superpotential of the charged lepton mass term is given in terms of modular forms of weight 2,  $\mathbf{Y}_3^{(2)}$ . It is given as:

$$w_E = \alpha_e e^c H_d \mathbf{Y}_3^{(2)} L + \beta_e \mu^c H_d \mathbf{Y}_3^{(2)} L + \gamma_e \tau^c H_d \mathbf{Y}_3^{(2)} L, \quad (3.1)$$

where  $L$  is the left-handed  $A_4$  triplet leptons. We can take real for  $\alpha_e$ ,  $\beta_e$  and  $\gamma_e$ . Under CP, the superfields transform as:

$$e^c \xrightarrow{CP} X_1^* \bar{e}^c, \quad \mu^c \xrightarrow{CP} X_{1''}^* \bar{\mu}^c, \quad \tau^c \xrightarrow{CP} X_{1'}^* \bar{\tau}^c, \quad L \xrightarrow{CP} X_3 \bar{L}, \quad H_d \xrightarrow{CP} \eta_d \bar{H}_d, \quad (3.2)$$

and we can take  $\eta_d = 1$  without loss of generality. Since the representations of  $S$  and  $T$  are symmetric as seen in eq. (2.11), we can choose  $X_3 = \mathbb{1}$  and  $X_1 = X_{1'} = X_{1''} = \mathbb{1}$ .

Taking  $(e_L, \mu_L, \tau_L)$  in the flavor base, the charged lepton mass matrix  $M_E$  is simply written as:

$$M_E(\tau) = v_d \begin{pmatrix} \alpha_e & 0 & 0 \\ 0 & \beta_e & 0 \\ 0 & 0 & \gamma_e \end{pmatrix} \begin{pmatrix} Y_1(\tau) & Y_3(\tau) & Y_2(\tau) \\ Y_2(\tau) & Y_1(\tau) & Y_3(\tau) \\ Y_3(\tau) & Y_2(\tau) & Y_1(\tau) \end{pmatrix}_{RL}, \quad (3.3)$$



where  $v_d$  is VEV of the neutral component of  $H_d$ , and coefficients  $\alpha_e, \beta_e$  and  $\gamma_e$  are taken to be real without loss of generality. Under CP transformation, the mass matrix  $M_E$  is transformed following from eq. (2.24) as:

$$M_E(\tau) \xrightarrow{CP} M_E(-\tau^*) = M_E^*(\tau) = v_d \begin{pmatrix} \alpha_e & 0 & 0 \\ 0 & \beta_e & 0 \\ 0 & 0 & \gamma_e \end{pmatrix} \begin{pmatrix} Y_1(\tau)^* & Y_3(\tau)^* & Y_2(\tau)^* \\ Y_2(\tau)^* & Y_1(\tau)^* & Y_3(\tau)^* \\ Y_3(\tau)^* & Y_2(\tau)^* & Y_1(\tau)^* \end{pmatrix}_{RL}. \quad (3.4)$$

Let us discuss the neutrino mass matrix. Suppose neutrinos to be Majorana particles. By using the Weinberg operator, the superpotential of the neutrino mass term,  $w_\nu$  is given as:

$$w_\nu = -\frac{1}{\Lambda} (H_u H_u L L \mathbf{Y}_r^{(4)})_1, \quad (3.5)$$

where  $\Lambda$  is a relevant cutoff scale. Since the left-handed lepton doublet has weight  $-2$ , the superpotential is given in terms of modular forms of weight 4,  $\mathbf{Y}_3^{(4)}$ ,  $\mathbf{Y}_1^{(4)}$  and  $\mathbf{Y}_{1'}^{(4)}$ .

By putting  $v_u$  for VEV of the neutral component of  $H_u$  and using the tensor products of  $A_4$  in appendix A, we have

$$\begin{aligned} w_\nu &= \frac{v_u^2}{\Lambda} \left[ \begin{pmatrix} 2\nu_e \nu_e - \nu_\mu \nu_\tau - \nu_\tau \nu_\mu \\ 2\nu_\tau \nu_\tau - \nu_e \nu_\mu - \nu_\mu \nu_\tau \\ 2\nu_\mu \nu_\mu - \nu_\tau \nu_e - \nu_e \nu_\tau \end{pmatrix} \otimes \mathbf{Y}_3^{(4)} \right. \\ &\quad \left. + (\nu_e \nu_e + \nu_\mu \nu_\tau + \nu_\tau \nu_\mu) \otimes g_1^\nu \mathbf{Y}_1^{(4)} + (\nu_e \nu_\tau + \nu_\mu \nu_\mu + \nu_\tau \nu_e) \otimes g_2^\nu \mathbf{Y}_{1'}^{(4)} \right] \\ &= \frac{v_u^2}{\Lambda} \left[ (2\nu_e \nu_e - \nu_\mu \nu_\tau - \nu_\tau \nu_\mu) Y_1^{(4)} + (2\nu_\tau \nu_\tau - \nu_e \nu_\mu - \nu_\mu \nu_e) Y_3^{(4)} + (2\nu_\mu \nu_\mu - \nu_\tau \nu_e - \nu_e \nu_\tau) Y_2^{(4)} \right. \\ &\quad \left. + (\nu_e \nu_e + \nu_\mu \nu_\tau + \nu_\tau \nu_\mu) g_1^\nu \mathbf{Y}_1^{(4)} + (\nu_e \nu_\tau + \nu_\mu \nu_\mu + \nu_\tau \nu_e) g_2^\nu \mathbf{Y}_{1'}^{(4)} \right], \quad (3.6) \end{aligned}$$

where  $\mathbf{Y}_3^{(4)}$ ,  $\mathbf{Y}_1^{(4)}$  and  $\mathbf{Y}_{1'}^{(4)}$  are given in eq. (B.6) of appendix B, and  $g_1^\nu, g_2^\nu$  are complex parameters in general. The neutrino mass matrix is written as follows:

$$M_\nu(\tau) = \frac{v_u^2}{\Lambda} \left[ \begin{pmatrix} 2Y_1^{(4)}(\tau) & -Y_3^{(4)}(\tau) & -Y_2^{(4)}(\tau) \\ -Y_3^{(4)}(\tau) & 2Y_2^{(4)}(\tau) & -Y_1^{(4)}(\tau) \\ -Y_2^{(4)}(\tau) & -Y_1^{(4)}(\tau) & 2Y_3^{(4)}(\tau) \end{pmatrix} + g_1^\nu \mathbf{Y}_1^{(4)}(\tau) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + g_2^\nu \mathbf{Y}_{1'}^{(4)}(\tau) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right], \quad (3.7)$$

which is the same one in ref. [75]. Under CP transformation, the mass matrix  $M_\nu$  is transformed following from eq. (2.24) as:

$$\begin{aligned} M_\nu(\tau) \xrightarrow{CP} M_\nu(-\tau^*) &= M_\nu^*(\tau) \\ &= \frac{v_u^2}{\Lambda} \left[ \begin{pmatrix} 2Y_1^{(4)*}(\tau) & -Y_3^{(4)*}(\tau) & -Y_2^{(4)*}(\tau) \\ -Y_3^{(4)*}(\tau) & 2Y_2^{(4)*}(\tau) & -Y_1^{(4)*}(\tau) \\ -Y_2^{(4)*}(\tau) & -Y_1^{(4)*}(\tau) & 2Y_3^{(4)*}(\tau) \end{pmatrix} + g_1^{\nu*} \mathbf{Y}_1^{(4)*}(\tau) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + g_2^{\nu*} \mathbf{Y}_{1'}^{(4)*}(\tau) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right]. \quad (3.8) \end{aligned}$$

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

$$\tau \xrightarrow{CP} -\tau^* = \tau, \tag{3.9}$$

which indicates  $\tau$  lies on the imaginary axis,  $\text{Re}[\tau] = 0$ . In addition to  $\text{Re}[\tau] = 0$ , CP is conserved at the boundary of the fundamental domain. Then, one has

$$M_E(\tau) = M_E^*(\tau), \quad M_\nu(\tau) = M_\nu^*(\tau), \tag{3.10}$$

which leads to  $g'_1$  and  $g'_2$  being real. Since parameters  $\alpha_e, \beta_e, \gamma_e$  are also real, the source of the CP violation is only non-trivial  $\text{Re}[\tau]$  after breaking the modular symmetry. In the next section, we present numerical analysis of the CP violation by investigating the value of the modulus  $\tau$ .

#### 4 Numerical results of leptonic CP violation

We have presented the CP invariant lepton mass matrices in the  $A_4$  modular symmetry. These mass matrices are the same ones in ref. [75] except for parameters  $g'_1$  and  $g'_2$  being real. If the CP violation will be confirmed at the experiments of neutrino oscillations, the CP symmetry should be broken spontaneously by VEV of the modulus  $\tau$ . Thus, VEV of  $\tau$  breaks the CP symmetry as well as the modular invariance. The source of the CP violation is only the real part of  $\tau$ . This situation is different from the previous work in ref. [75], where imaginary parts of  $g'_1$  and  $g'_2$  also break the CP symmetry explicitly. Our phenomenological concern is whether the spontaneous CP violation is realized due to the value of  $\tau$ , which is consistent with observed lepton mixing angles and neutrino masses. If this is the case, the CP violating Dirac phase and Majorana phases are predicted clearly under the fixed value of  $\tau$ .

Parameter ratios  $\alpha_e/\gamma_e$  and  $\beta_e/\gamma_e$  are given in terms of charged lepton masses and  $\tau$  as shown in appendix C. Therefore, the lepton mixing angles, the Dirac phase and Majorana phases are given by our model parameters  $g'_1$  and  $g'_2$  in addition to the value of  $\tau$ .

As the input charged lepton masses, we take Yukawa couplings of charged leptons at the GUT scale  $2 \times 10^{16}$  GeV, where  $\tan \beta = 5$  is taken as a bench mark [115, 116]:

$$y_e = (1.97 \pm 0.024) \times 10^{-6}, \quad y_\mu = (4.16 \pm 0.050) \times 10^{-4}, \quad y_\tau = (7.07 \pm 0.073) \times 10^{-3}, \tag{4.1}$$

where lepton masses are given by  $m_\ell = y_\ell v_H$  with  $v_H = 174$  GeV.

We also input the lepton mixing angles and neutrino mass parameters which are given by NuFit 5.0 in table 2 [117]. In our analysis,  $\delta_{CP}$  is output because its observed range is too wide at  $3\sigma$  confidence level. We investigate two possible cases of neutrino masses  $m_i$ , which are the normal hierarchy (NH),  $m_3 > m_2 > m_1$ , and the inverted hierarchy (IH),  $m_2 > m_1 > m_3$ . Neutrino masses and the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix  $U_{PMNS}$  [95, 96] are obtained by diagonalizing  $M_E^\dagger M_E$  and  $M_\nu^\dagger M_\nu$ . We also investigate the

observable	best fit $\pm 1 \sigma$ for NH	best fit $\pm 1 \sigma$ for IH
$\sin^2 \theta_{12}$	$0.304^{+0.012}_{-0.012}$	$0.304^{+0.013}_{-0.012}$
$\sin^2 \theta_{23}$	$0.573^{+0.016}_{-0.020}$	$0.575^{+0.016}_{-0.019}$
$\sin^2 \theta_{13}$	$0.02219^{+0.00062}_{-0.00063}$	$0.02238^{+0.00063}_{-0.00062}$
$\Delta m_{\text{sol}}^2$	$7.42^{+0.21}_{-0.20} \times 10^{-5} \text{eV}^2$	$7.42^{+0.21}_{-0.20} \times 10^{-5} \text{eV}^2$
$\Delta m_{\text{atm}}^2$	$2.517^{+0.026}_{-0.028} \times 10^{-3} \text{eV}^2$	$-2.498^{+0.028}_{-0.028} \times 10^{-3} \text{eV}^2$

**Table 2.** The best fit  $\pm 1 \sigma$  of neutrino parameters from NuFIT 5.0 for NH and IH [117].

effective mass for the  $0\nu\beta\beta$  decay,  $\langle m_{ee} \rangle$  (see appendix D) and the sum of three neutrino masses  $\sum m_i$  since it is constrained by the recent cosmological data, which is the upper-bound  $\sum m_i \leq 120 \text{meV}$  obtained at the 95% confidence level [118, 119].

### 4.1 Case of normal hierarchy of neutrino masses

Let us discuss numerical results for NH of neutrino masses. The ratios  $\alpha_e/\gamma_e$  and  $\beta_e/\gamma_e$  are given after fixing charged lepton masses and  $\tau$  as shown in appendix C. However, in practice, we scan  $\alpha_e/\gamma_e$  and  $\beta_e/\gamma_e$  to obtain the observed charged lepton mass ratio and include them in  $\chi^2$  fit as well as three mixing angles and  $\Delta m_{\text{atm}}^2/\Delta m_{\text{sol}}^2$ .

We have already studied the lepton mass matrices in eqs. (3.3) and (3.7) phenomenologically at the nearby fixed points of the modulus because the spontaneous CP violation in Type IIB string theory is possibly realized at nearby fixed points, where the moduli stabilization is performed in a controlled way [120, 121]. There are two fixed points in the fundamental domain of  $\text{PSL}(2, \mathbb{Z})$ ,  $\tau = i$  and  $\tau = \omega$ . Indeed, the viable  $\tau$  of our lepton mass matrices is found around  $\tau = i$  [75].

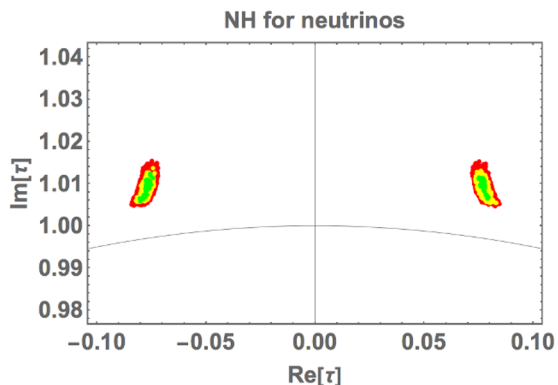
Based on this result of ref. [75], we scan  $\tau$  around  $i$  while neutrino couplings  $g_1'$  and  $g_2'$  are scanned in the real space of  $[-10, 10]$ . As a measure of good-fit, we adopt the sum of one-dimensional  $\chi^2$  function for four accurately known dimensionless observables  $\Delta m_{\text{atm}}^2/\Delta m_{\text{sol}}^2$ ,  $\sin^2 \theta_{12}$ ,  $\sin^2 \theta_{23}$  and  $\sin^2 \theta_{13}$  in NuFit 5.0 [117]. In addition, we employ Gaussian approximations for fitting  $m_e/m_\tau$  and  $m_\mu/m_\tau$  by using the data of PDG [122].

In figure 1 we show the allowed region on the  $\text{Re}[\tau] - \text{Im}[\tau]$  plane, where three mixing angles and  $\Delta m_{\text{atm}}^2/\Delta m_{\text{sol}}^2$  are consistent with observed ones. The green, yellow and red regions correspond to  $2\sigma$ ,  $3\sigma$  and  $5\sigma$  confidence levels, respectively.

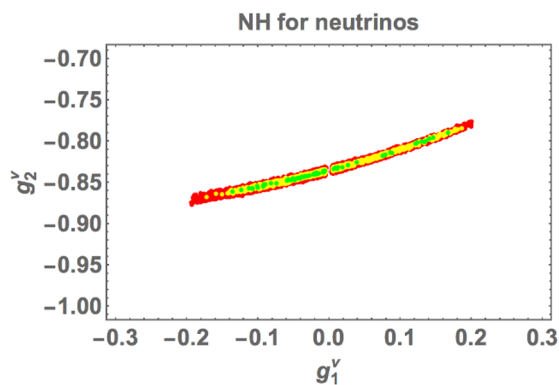
The allowed region of  $\tau$  is restricted in the narrow regions. This result is contrast to the previous one in ref. [75], where non-trivial phases of  $g_1'$  and  $g_2'$  enlarged the allowed region of  $\tau$ . The predicted range of  $\tau$  is in  $\text{Re}[\tau] = \pm[0.073, 0.083]$  and  $\text{Im}[\tau] = [1.006, 1.014]$  at  $3\sigma$  confidence level (yellow), which are close to the fixed point  $\tau = i$ .

The allowed region of  $g_1'$  and  $g_2'$  is also shown in figure 2, where  $g_1'$  is in the rather wide region of  $[-0.18, 0.18]$  while  $g_2'$  is restricted in  $[-0.87, -0.79]$  at  $3\sigma$  confidence level (yellow).

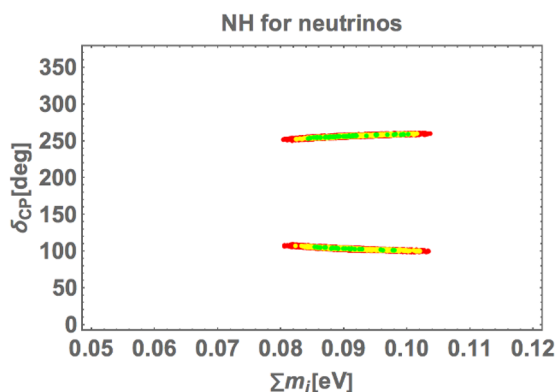
Due to restricted  $\text{Re}[\tau]$ , the CP violating Dirac phase  $\delta_{\text{CP}}$ , which is defined in appendix D, is predicted clearly. In figure 3, we show prediction of  $\delta_{\text{CP}}$  versus the sum of neutrino masses  $\sum m_i$ . It is remarked that  $\delta_{\text{CP}}$  is almost independent of  $\sum m_i$ . The pre-



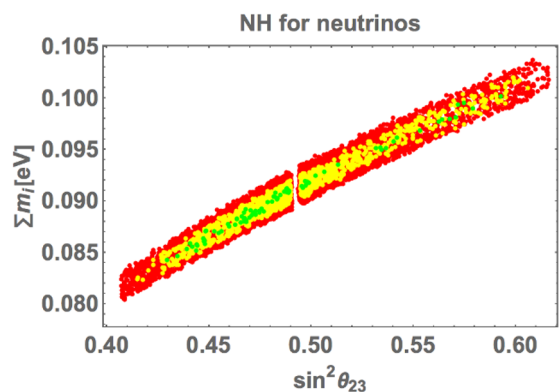
**Figure 1.** Allowed regions of  $\tau$  for NH. Green, yellow and red correspond to  $2\sigma$ ,  $3\sigma$ ,  $5\sigma$  confidence levels, respectively. The solid curve is the boundary of the fundamental domain,  $|\tau| = 1$ .



**Figure 2.** The allowed region of  $g_1^\nu$  and  $g_2^\nu$ , which are real parameters, for NH. Colors denote same ones in figure 1.



**Figure 3.** The prediction of  $\delta_{CP}$  versus  $\sum m_i$  for NH. Colors denote same ones in figure 1.



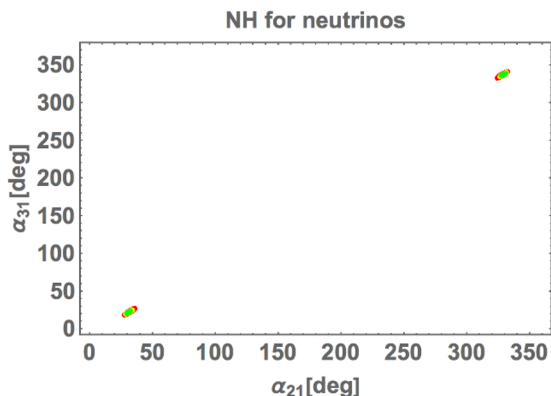
**Figure 4.** The allowed region on  $\sin^2 \theta_{23} - \sum m_i$  plane for NH.

dicted ranges of  $\delta_{CP}$  are narrow such as  $[98^\circ, 110^\circ]$  and  $[250^\circ, 262^\circ]$  at  $3\sigma$  confidence level (yellow). The predicted ranges  $[98^\circ, 110^\circ]$  and  $[250^\circ, 262^\circ]$  correspond to  $\text{Re}[\tau] = (0.073-0.083)$  and  $\text{Re}[\tau] = -(0.073-0.083)$ , respectively. The predicted  $\sum m_i$  is in  $[82, 102]$  meV for  $3\sigma$  confidence level (yellow). The minimal cosmological model,  $\Lambda\text{CDM} + \sum m_i$ , provides the upper-bound  $\sum m_i < 120$  meV [118, 119]. Thus, our predicted sum of neutrino masses is consistent with the cosmological bound 120 meV.

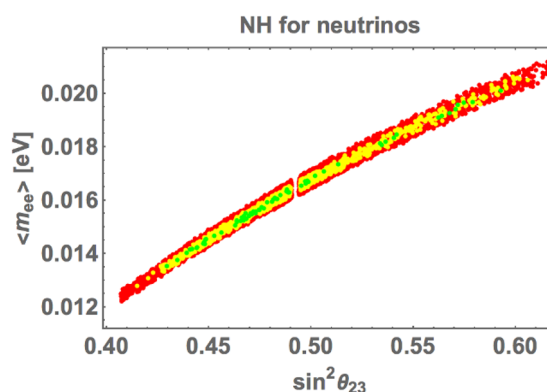
In figure 4, we show the allowed region on the  $\sin^2 \theta_{23} - \sum m_i$  plane. Since  $\sum m_i$  depends on the value of  $\sin^2 \theta_{23}$  significantly, the crucial test of our prediction will be available in the near future.

In figure 5, we show the prediction of Majorana phases  $\alpha_{21}$  and  $\alpha_{31}$ , which are defined by appendix D. The predicted  $[\alpha_{21}, \alpha_{31}]$  are around  $[30^\circ, 20^\circ]$  and  $[330^\circ, 340^\circ]$  since the source of the CP violation,  $\text{Re}[\tau]$  is in the narrow range  $\text{Re}[\tau] = \pm[0.073, 0.083]$ .

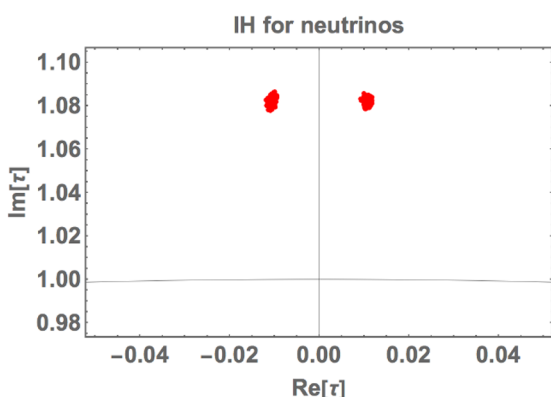
We can calculate the effective mass  $\langle m_{ee} \rangle$  for the  $0\nu\beta\beta$  decay by using the Dirac phase and Majorana phases as seen in appendix D. We show the predicted value of  $\langle m_{ee} \rangle$  versus  $\sin^2 \theta_{23}$  as seen in figure 6. The predicted  $\langle m_{ee} \rangle$  is in  $[12.5, 20.5]$  meV for  $3\sigma$  confidence



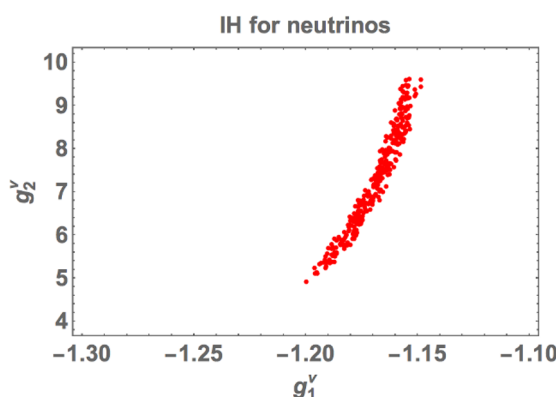
**Figure 5.** Predicted Majorana phases  $\alpha_{21}$  and  $\alpha_{31}$  for NH. Colors denote same ones in figure 1.



**Figure 6.** The predicted  $\langle m_{ee} \rangle$  versus  $\sin^2 \theta_{23}$  for NH. Colors denote same ones in figure 1.



**Figure 7.** Allowed regions of  $\tau$  for IH. Red corresponds to  $5\sigma$  confidence level.



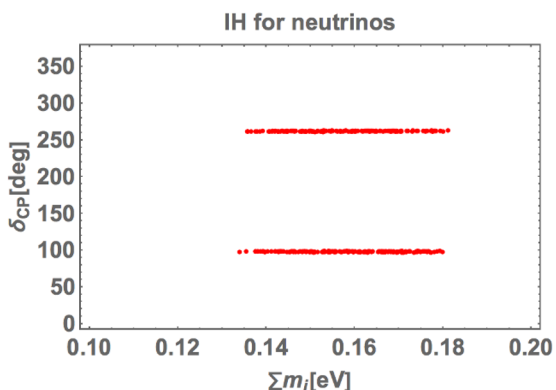
**Figure 8.** The allowed region of  $g'_1$  and  $g'_2$ , which are real parameters, for IH.

level (yellow). The prediction of  $\langle m_{ee} \rangle \simeq 20$  meV will be testable in the future experiments of the neutrinoless double beta decay.

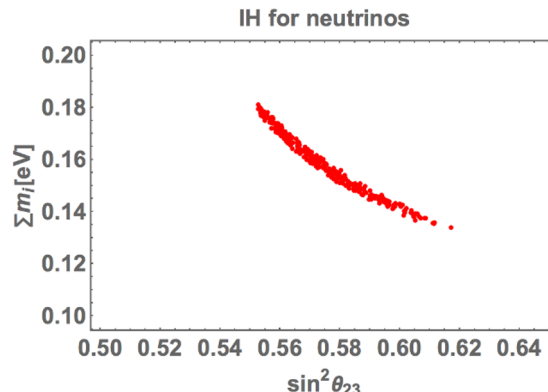
It is important to understand the difference between the results in the present paper and the previous ones in ref. [75], where imaginary parts of  $g'_1$  and  $g'_2$  also break the CP symmetry explicitly. The modulus  $\tau$  is severely restricted around  $\text{Re}[\tau] = \pm 0.08$  and  $\text{Im}[\tau] = 1.01$  in this work while it is allowed in rather wide region in the previous work. Indeed, the smaller  $\text{Re}[\tau]$  and the larger  $\text{Im}[\tau]$  are allowed such as  $\text{Re}[\tau] \simeq \pm 0.03$  and  $\text{Im}[\tau] \simeq 1.1$  in the previous results. Due to this restricted  $\tau$  in this work,  $\delta_{\text{CP}}$  and the sum of neutrino masses  $\sum m_i$  are predicted clearly. On the other hand, the CP conservation is still allowed and  $\sum m_i$  could be larger than 120 meV in the previous work. Moreover, the Dirac phase  $\delta_{\text{CP}}$  depends on  $\sum m_i$ .

## 4.2 Case of inverted hierarchy of neutrino masses

We discuss the case of IH of neutrino masses. In figure 7, we show the allowed region on the  $\text{Re}[\tau]$ – $\text{Im}[\tau]$  plane, where the red region corresponds to  $5\sigma$  confidence level like in figure 1. However, there are no green and yellow regions of  $2\sigma$  and  $3\sigma$  confidence levels.



**Figure 9.** The prediction of  $\delta_{\text{CP}}$  versus  $\sum m_i$  for IH.



**Figure 10.** The allowed region on  $\sin^2 \theta_{23}$ – $\sum m_i$  plane for IH.

The range of  $\tau$  is in  $\text{Re}[\tau] = \pm[0.009, 0.012]$  and  $\text{Im}[\tau] = [1.076, 1.087]$  at  $5\sigma$  confidence level, which are close to  $\tau = i$ .

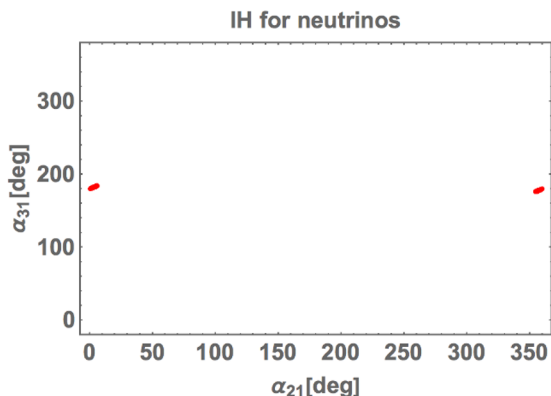
The allowed region of  $g'_1$  and  $g'_2$  is also shown in figure 8, where  $g'_1$  is restricted in the narrow range of  $[-1.20, -1.15]$  while  $g'_2$  is rather large as in  $[4.8, 9.6]$  for  $5\sigma$ .

In figure 9, we show prediction of  $\delta_{\text{CP}}$  versus  $\sum m_i$ . It is remarked that  $\delta_{\text{CP}}$  is almost independent of  $\sum m_i$ . The predicted range of  $\delta_{\text{CP}}$  is in  $[95^\circ, 100^\circ]$  and  $[260^\circ, 265^\circ]$  at  $5\sigma$  confidence level while the sum of neutrino masses are in the range of  $[134, 180]$  meV. In our numerical result, there is no region of the sum of neutrino masses less than 120 meV. The upper-bound of the minimal cosmological model,  $\Lambda\text{CDM} + \sum m_i$ , is  $\sum m_i < 120$  meV [118, 119], however, it becomes weaker when the data are analysed in the context of extended cosmological models [122]. The predicted sum of neutrino masses of IH may be still consistent with the cosmological bound.

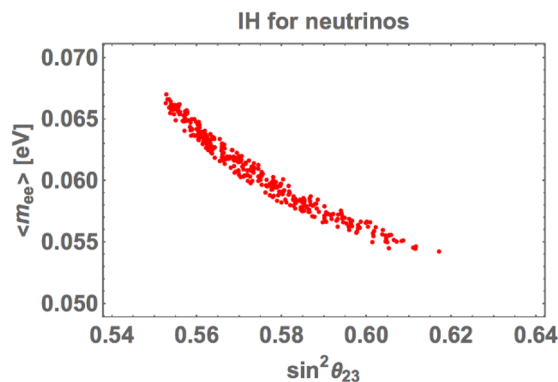
We show the allowed region on the  $\sum m_i$ – $\sin^2 \theta_{23}$  plane in figure 10. The precise measurement of  $\sin^2 \theta_{23}$  will provide a severe test for our prediction since  $\sin^2 \theta_{23} > 0.55$  is obtained for IH.

In figure 11, we show the prediction of Majorana phases  $\alpha_{21}$  and  $\alpha_{31}$ . The predicted  $[\alpha_{21}, \alpha_{31}]$  are restricted around  $[3^\circ, 182^\circ]$  and  $[356^\circ, 178^\circ]$ . We also show the predicted value of  $\langle m_{ee} \rangle$  versus  $\sin^2 \theta_{23}$  as seen in figure 12. The predicted  $\langle m_{ee} \rangle$  is in  $[54, 67]$  meV for  $5\sigma$  confidence level.

As well as the case of NH, we comment on the difference between the results in the present paper and the previous ones in ref. [75], where  $g'_1$  and  $g'_2$  are complex. Our results are obtained at more than  $3\sigma$  confidence level, on the other hand, the previous ones are at less than  $3\sigma$  confidence level. The modulus  $\tau$  is also severely restricted in this work while it is allowed in rather wide region in the previous work. The sum of neutrino masses  $\sum m_i$  is larger than 120 meV in this work, on the other hand, it is allowed to be smaller than 120 meV in the previous work. For example, it could be 90 meV, and the Dirac phase  $\delta_{\text{CP}}$  depends on  $\sum m_i$ .



**Figure 11.** Predicted Majorana phases  $\alpha_{21}$  and  $\alpha_{31}$  for IH.



**Figure 12.** The predicted  $\langle m_{ee} \rangle$  versus  $\sin^2 \theta_{23}$  for IH.

	NH	IH
$\tau$	$-0.0796 + 1.0065 i$	$0.0103 + 1.0812 i$
$g_1'$	0.124	-1.17
$g_2'$	-0.802	6.79
$\alpha_e/\gamma_e$	$6.82 \times 10^{-2}$	$6.76 \times 10^{-2}$
$\beta_e/\gamma_e$	$1.02 \times 10^{-3}$	$1.02 \times 10^{-3}$
$\sin^2 \theta_{12}$	0.290	0.291
$\sin^2 \theta_{23}$	0.564	0.579
$\sin^2 \theta_{13}$	0.0225	0.0219
$\delta_{\text{CP}}^\ell$	$258^\circ$	$262^\circ$
$[\alpha_{21}, \alpha_{31}]$	$[330^\circ, 338^\circ]$	$[3.24^\circ, 182^\circ]$
$\sum m_i$	97.9 meV	153 meV
$\langle m_{ee} \rangle$	19.2 meV	59.1 meV
$\chi^2$	1.98	4.12

**Table 3.** Numerical values of parameters and observables at the sample points of NH and IH.

### 4.3 Parameter samples of NH and IH

We show the numerical result of two samples for NH and IH, respectively. In table 3, parameters and outputs of our calculations are presented for both NH and IH.

We also present the mixing matrices of charged leptons  $U_E$  and neutrinos  $U_\nu$  for the samples of table 3. For NH, those are:

$$\begin{aligned}
 U_E &\approx \begin{pmatrix} 0.983 & -0.020 + 0.158 i & -0.011 + 0.092 i \\ 0.016 + 0.130 i & 0.958 & -0.255 + 0.001 i \\ 0.016 + 0.129 i & 0.239 + 0.001 i & 0.962 \end{pmatrix}, \\
 U_\nu &\approx \begin{pmatrix} 0.838 & -0.541 + 0.068 i & -0.008 + 0.031 i \\ 0.450 + 0.076 i & 0.688 & 0.564 - 0.0008 i \\ -0.299 - 0.021 i & -0.478 - 0.020 i & 0.825 \end{pmatrix},
 \end{aligned} \tag{4.2}$$

which are given in the diagonal base of the generator  $S$  in order to see the hierarchical structure of flavor mixing [75]. The PMNS mixing matrix is given as  $U_{\text{PMNS}} = U_E^\dagger U_\nu$ . The diagonal base of  $S$  is obtained by using the following unitary matrix:

$$V_S \equiv \begin{pmatrix} -\frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}, \quad (4.3)$$

which leads to  $V_S S V_S^\dagger = \text{diag}(1, -1, -1)$  [75]. Then, the charged lepton and neutrino mass matrices are transformed as  $V_S M_f^\dagger M_f V_S^\dagger$  ( $f = E, \nu$ ).

For IH, the mixing matrices are:

$$\begin{aligned} U_E &\approx \begin{pmatrix} 0.983 & 0.155 + 0.019i & 0.091 + 0.011i \\ 0.127 + 0.015i & 0.956 & -0.264 - 0.001i \\ -0.128 + 0.016 & 0.248 - 0.001i & 0.960 \end{pmatrix}, \\ U_\nu &\approx \begin{pmatrix} 0.840 & 0.0007 + 0.542i & 0.032 - 0.001i \\ -0.022 + 0.445i & 0.691 & 0.570 - 0.002i \\ -0.016 - 0.310i & -0.478 - 0.023i & 0.821 \end{pmatrix}, \end{aligned} \quad (4.4)$$

which are also given in the diagonal base of the generator  $S$ .

For both NH and IH, the mixing matrix of charged leptons  $U_E$  is hierarchical one, on the other hand, two large mixing angles of 1–2 and 2–3 flavors appear in the neutrino mixing matrix  $U_\nu$ .

In our numerical calculations, we have not included the RGE effects in the lepton mixing angles and neutrino mass ratio  $\Delta m_{\text{sol}}^2 / \Delta m_{\text{atm}}^2$ . We suppose that those corrections are very small between the electroweak and GUT scales. This assumption is justified well in the case of  $\tan \beta \leq 5$  unless neutrino masses are almost degenerate [27].

## 5 Summary and discussions

The modular invariant  $A_4$  model of lepton flavors has been studied combining with the generalized CP symmetry. In our model, both CP and modular symmetries are broken spontaneously by VEV of the modulus  $\tau$ . The source of the CP violation is a non-trivial value of  $\text{Re}[\tau]$  while parameters of neutrinos  $g_1'$  and  $g_2'$  are real.

We have found allowed region of  $\tau$  close to the fixed point  $\tau = i$ , which is consistent with the observed lepton mixing angles and lepton masses for NH at  $2\sigma$  confidence level. The CP violating Dirac phase  $\delta_{\text{CP}}$  is predicted clearly in  $[98^\circ, 110^\circ]$  and  $[250^\circ, 262^\circ]$  at  $3\sigma$  confidence level. The predicted  $\sum m_i$  is in  $[82, 102]$  meV with  $3\sigma$  confidence level.

There is also allowed region of  $\tau$  close to the fixed point  $\tau = i$  for IH at  $5\sigma$  confidence level. The predicted  $\delta_{\text{CP}}$  is in  $[95^\circ, 100^\circ]$  and  $[260^\circ, 265^\circ]$  at  $5\sigma$  confidence level. The sum of neutrino masses is predicted in  $\sum m_i = [134, 180]$  meV.



By using the predicted Dirac phase and the Majorana phases, we have obtained the effective mass  $\langle m_{ee} \rangle$  for the  $0\nu\beta\beta$  decay, which are in [12.5, 20.5] meV for NH at  $3\sigma$  confidence level and in [54, 67] meV for IH at  $5\sigma$  confidence level. Since KamLAND-Zen experiment [123] presented the upper bound on the effective Majorana mass as  $\langle m_{ee} \rangle < 61\text{--}165$  meV by using a variety of nuclear matrix element calculations, the prediction of [54, 67] meV for IH will be tested in the near future. Furthermore, the prediction of  $\langle m_{ee} \rangle \simeq 20$  meV for NH will be also testable in the future experiments of the neutrinoless double beta decay.

Since the CP symmetry is conserved at the boundary of the fundamental domain, one may expect the size of CP violation to be small at the nearby fixed point of  $\tau = i$ . In order to estimate of the size of CP violation, we can calculate the rephasing invariant CP violating measure of leptons,  $J_{CP}$  [124, 125] from mass matrices directly [126]. By using approximate forms of lepton mass matrices at nearby fixed points in ref. [75], we have obtained the relation between the magnitude of  $J_{CP}$  and the deviation from  $\tau = i$  semi-quantitatively. In order to reproduce the almost maximal size  $|J_{CP}| = 0.03$ , it is enough to take  $\epsilon = \pm\mathcal{O}(0.05)$  where  $\epsilon$  is supposed to be real in the definition of  $\tau = i + \epsilon$ . Since it is important to study CP violation at nearby fixed points comprehensively, we will present appropriate forms in another paper.

In our model, the modulus  $\tau$  dominates the CP violation. Therefore, the determination of  $\tau$  is the most important work. Although we have constrained  $\tau$  by observables of leptons phenomenologically, one also should pay attention to the recent theoretical work of the moduli stabilization from the viewpoint of modular flavor symmetries [127]. The study of modulus  $\tau$  is interesting to reveal the flavor theory in both theoretical and phenomenological aspects.

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## A Tensor product of $A_4$ group

We take the generators of  $A_4$  group for the triplet as follows:

$$S = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \quad (\text{A.1})$$

where  $\omega = e^{i\frac{2}{3}\pi}$  for a triplet. In this base, the multiplication rule is

$$\begin{aligned} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}_{\mathbf{3}} \otimes \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}_{\mathbf{3}} &= (a_1b_1 + a_2b_3 + a_3b_2)_{\mathbf{1}} \oplus (a_3b_3 + a_1b_2 + a_2b_1)_{\mathbf{1}'} \\ &\oplus (a_2b_2 + a_1b_3 + a_3b_1)_{\mathbf{1}''} \\ &\oplus \frac{1}{3} \begin{pmatrix} 2a_1b_1 - a_2b_3 - a_3b_2 \\ 2a_3b_3 - a_1b_2 - a_2b_1 \\ 2a_2b_2 - a_1b_3 - a_3b_1 \end{pmatrix}_{\mathbf{3}} \oplus \frac{1}{2} \begin{pmatrix} a_2b_3 - a_3b_2 \\ a_1b_2 - a_2b_1 \\ a_3b_1 - a_1b_3 \end{pmatrix}_{\mathbf{3}}, \\ \mathbf{1} \otimes \mathbf{1} &= \mathbf{1}, \quad \mathbf{1}' \otimes \mathbf{1}' = \mathbf{1}'', \quad \mathbf{1}'' \otimes \mathbf{1}'' = \mathbf{1}', \quad \mathbf{1}' \otimes \mathbf{1}'' = \mathbf{1}, \end{aligned} \tag{A.2}$$

where

$$T(\mathbf{1}') = \omega, \quad T(\mathbf{1}'') = \omega^2. \tag{A.3}$$

More details are shown in the review [6, 7].

## B Modular forms in $A_4$ symmetry

For  $\Gamma_3 \simeq A_4$ , the dimension of the linear space  $\mathcal{M}_k(\Gamma(3))$  of modular forms of weight  $k$  is  $k + 1$  [112–114], i.e., there are three linearly independent modular forms of the lowest non-trivial weight 2. These forms have been explicitly obtained [22] in terms of the Dedekind eta-function  $\eta(\tau)$ :

$$\eta(\tau) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n), \quad q = \exp(i2\pi\tau), \tag{B.1}$$

where  $\eta(\tau)$  is a so called modular form of weight 1/2. In what follows we will use the following base of the  $A_4$  generators  $S$  and  $T$  in the triplet representation:

$$S = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \tag{B.2}$$

where  $\omega = \exp(i\frac{2}{3}\pi)$ . The modular forms of weight 2 ( $k = 2$ ) transforming as a triplet of  $A_4$ ,  $\mathbf{Y}_3^{(2)}(\tau) = (Y_1(\tau) Y_2(\tau), Y_3(\tau))^T$ , can be written in terms of  $\eta(\tau)$  and its derivative [22]:

$$\begin{aligned} Y_1(\tau) &= \frac{i}{2\pi} \left( \frac{\eta'(\tau/3)}{\eta(\tau/3)} + \frac{\eta'((\tau+1)/3)}{\eta((\tau+1)/3)} + \frac{\eta'((\tau+2)/3)}{\eta((\tau+2)/3)} - \frac{27\eta'(3\tau)}{\eta(3\tau)} \right), \\ Y_2(\tau) &= \frac{-i}{\pi} \left( \frac{\eta'(\tau/3)}{\eta(\tau/3)} + \omega^2 \frac{\eta'((\tau+1)/3)}{\eta((\tau+1)/3)} + \omega \frac{\eta'((\tau+2)/3)}{\eta((\tau+2)/3)} \right), \\ Y_3(\tau) &= \frac{-i}{\pi} \left( \frac{\eta'(\tau/3)}{\eta(\tau/3)} + \omega \frac{\eta'((\tau+1)/3)}{\eta((\tau+1)/3)} + \omega^2 \frac{\eta'((\tau+2)/3)}{\eta((\tau+2)/3)} \right). \end{aligned} \tag{B.3}$$

The overall coefficient in eq. (B.3) is one possible choice. It cannot be uniquely determined. The triplet modular forms of weight 2 have the following  $q$ -expansions:

$$\mathbf{Y}_3^{(2)}(\tau) = \begin{pmatrix} Y_1(\tau) \\ Y_2(\tau) \\ Y_3(\tau) \end{pmatrix} = \begin{pmatrix} 1 + 12q + 36q^2 + 12q^3 + \dots \\ -6q^{1/3}(1 + 7q + 8q^2 + \dots) \\ -18q^{2/3}(1 + 2q + 5q^2 + \dots) \end{pmatrix}. \quad (\text{B.4})$$

They satisfy also the constraint [22]:

$$Y_2(\tau)^2 + 2Y_1(\tau)Y_3(\tau) = 0. \quad (\text{B.5})$$

The modular forms of the higher weight,  $k$ , can be obtained by the  $A_4$  tensor products of the modular forms with weight 2,  $\mathbf{Y}_3^{(2)}(\tau)$ , as given in appendix A. For weight 4, that is  $k = 4$ , there are five modular forms by the tensor product of  $\mathbf{3} \otimes \mathbf{3}$  as:

$$\begin{aligned} \mathbf{Y}_{\mathbf{1}}^{(4)}(\tau) &= Y_1(\tau)^2 + 2Y_2(\tau)Y_3(\tau), & \mathbf{Y}_{\mathbf{1}'}^{(4)}(\tau) &= Y_3(\tau)^2 + 2Y_1(\tau)Y_2(\tau), \\ \mathbf{Y}_{\mathbf{1}''}^{(4)}(\tau) &= Y_2(\tau)^2 + 2Y_1(\tau)Y_3(\tau) = 0, & \mathbf{Y}_{\mathbf{3}}^{(4)}(\tau) &= \begin{pmatrix} Y_1^{(4)}(\tau) \\ Y_2^{(4)}(\tau) \\ Y_3^{(4)}(\tau) \end{pmatrix} = \begin{pmatrix} Y_1(\tau)^2 - Y_2(\tau)Y_3(\tau) \\ Y_3(\tau)^2 - Y_1(\tau)Y_2(\tau) \\ Y_2(\tau)^2 - Y_1(\tau)Y_3(\tau) \end{pmatrix}, \end{aligned} \quad (\text{B.6})$$

where  $\mathbf{Y}_{\mathbf{1}''}^{(4)}(\tau)$  vanishes due to the constraint of eq. (B.5).

### C Determination of $\alpha_e/\gamma_e$ and $\beta_e/\gamma_e$

The coefficients  $\alpha_e$ ,  $\beta_e$ , and  $\gamma_e$  in eq. (3.3) are taken to be real positive without loss of generality. We show these parameters are described in terms of the modular parameter  $\tau$  and the charged lepton masses. We rewrite the mass matrix of eq. (3.3) as

$$M_E = v_d \gamma_e \begin{pmatrix} \hat{\alpha}_e & 0 & 0 \\ 0 & \hat{\beta}_e & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} Y_1(\tau) & Y_3(\tau) & Y_2(\tau) \\ Y_2(\tau) & Y_1(\tau) & Y_3(\tau) \\ Y_3(\tau) & Y_2(\tau) & Y_1(\tau) \end{pmatrix}, \quad (\text{C.1})$$

where  $\hat{\alpha}_e \equiv \alpha_e/\gamma_e$  and  $\hat{\beta}_e \equiv \beta_e/\gamma_e$ . Denoting charged lepton masses  $m_1 = m_e$ ,  $m_2 = m_\mu$  and  $m_3 = m_\tau$ , we have three equations as:

$$\sum_{i=1}^3 m_i^2 = \text{Tr}[M_E^\dagger M_E] = v_d^2 \gamma_e^2 (1 + \hat{\alpha}_e^2 + \hat{\beta}_e^2) C_1^e, \quad (\text{C.2})$$

$$\prod_{i=1}^3 m_i^2 = \text{Det}[M_E^\dagger M_E] = v_d^6 \gamma_e^6 \hat{\alpha}_e^2 \hat{\beta}_e^2 C_2^e, \quad (\text{C.3})$$

$$\chi = \frac{\text{Tr}[M_E^\dagger M_E]^2 - \text{Tr}[(M_E^\dagger M_E)^2]}{2} = v_d^4 \gamma_e^4 (\hat{\alpha}_e^2 + \hat{\alpha}_e^2 \hat{\beta}_e^2 + \hat{\beta}_e^2) C_3^e, \quad (\text{C.4})$$

where  $\chi \equiv m_1^2 m_2^2 + m_2^2 m_3^2 + m_3^2 m_1^2$ . The coefficients  $C_1^e$ ,  $C_2^e$  and  $C_3^e$  depend only on  $Y_i(\tau)$ 's, where  $Y_i(\tau)$ 's are determined if the value of modulus  $\tau$  is fixed. Those are given explicitly

as follows:

$$\begin{aligned}
 C_1^e &= |Y_1(\tau)|^2 + |Y_2(\tau)|^2 + |Y_3(\tau)|^2, \\
 C_2^e &= |Y_1(\tau)|^3 + |Y_2(\tau)|^3 + |Y_3(\tau)|^3 - 3Y_1(\tau)Y_2(\tau)Y_3(\tau)^2, \\
 C_3^e &= |Y_1(\tau)|^4 + |Y_2(\tau)|^4 + |Y_3(\tau)|^4 + |Y_1(\tau)Y_2(\tau)|^2 + |Y_2(\tau)Y_3(\tau)|^2 + |Y_1(\tau)Y_3(\tau)|^2 \\
 &\quad - 2\text{Re} \left[ Y_1^*(\tau)Y_2^*(\tau)Y_3^2(\tau) + Y_1^2(\tau)Y_2^*(\tau)Y_3^*(\tau) + Y_1^*(\tau)Y_2^2(\tau)Y_3^*(\tau) \right].
 \end{aligned}$$

Then, we obtain two equations which describe  $\hat{\alpha}_e$  and  $\hat{\beta}_e$  in terms of masses and  $\tau$ :

$$\frac{(1+s)(s+t)}{t} = \frac{(\sum m_i^2/C_1^e)(\chi/C_3^e)}{\prod m_i^2/C_2^e}, \quad \frac{(1+s)^2}{s+t} = \frac{(\sum m_i^2/C_1^e)^2}{\chi/C_3^e}, \quad (\text{C.5})$$

where we redefine the parameters  $\hat{\alpha}_e^2 + \hat{\beta}_e^2 = s$  and  $\hat{\alpha}_e^2 \hat{\beta}_e^2 = t$ . After fixing charged lepton masses and  $\tau$ , we obtain  $s$  and  $t$  numerically. They are related as follows:

$$\hat{\alpha}_e^2 = \frac{s \pm \sqrt{s^2 - 4t}}{2}, \quad \hat{\beta}_e^2 = \frac{s \mp \sqrt{s^2 - 4t}}{2}. \quad (\text{C.6})$$

## D Majorana and Dirac phases and $\langle m_{ee} \rangle$ in $0\nu\beta\beta$ decay

Supposing neutrinos to be Majorana particles, the PMNS matrix  $U_{\text{PMNS}}$  [95, 96] is parametrized in terms of the three mixing angles  $\theta_{ij}$  ( $i, j = 1, 2, 3$ ;  $i < j$ ), one CP violating Dirac phase  $\delta_{\text{CP}}$  and two Majorana phases  $\alpha_{21}, \alpha_{31}$  as follows:

$$U_{\text{PMNS}} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta_{\text{CP}}} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta_{\text{CP}}} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta_{\text{CP}}} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta_{\text{CP}}} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta_{\text{CP}}} & c_{23}c_{13} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\frac{\alpha_{21}}{2}} & 0 \\ 0 & 0 & e^{i\frac{\alpha_{31}}{2}} \end{pmatrix}, \quad (\text{D.1})$$

where  $c_{ij}$  and  $s_{ij}$  denote  $\cos\theta_{ij}$  and  $\sin\theta_{ij}$ , respectively.

The rephasing invariant CP violating measure of leptons [124, 125] is defined by the PMNS matrix elements  $U_{\alpha i}$ . It is written in terms of the mixing angles and the CP violating phase as:

$$J_{\text{CP}} = \text{Im} \left[ U_{e1}U_{\mu 2}U_{e2}^*U_{\mu 1}^* \right] = s_{23}c_{23}s_{12}c_{12}s_{13}c_{13}^2 \sin\delta_{\text{CP}}, \quad (\text{D.2})$$

where  $U_{\alpha i}$  denotes the each component of the PMNS matrix.

There are also other invariants  $I_1$  and  $I_2$  associated with Majorana phases

$$I_1 = \text{Im} [U_{e1}^*U_{e2}] = c_{12}s_{12}c_{13}^2 \sin\left(\frac{\alpha_{21}}{2}\right), \quad I_2 = \text{Im} [U_{e1}^*U_{e3}] = c_{12}s_{13}c_{13} \sin\left(\frac{\alpha_{31}}{2} - \delta_{\text{CP}}\right). \quad (\text{D.3})$$

We can calculate  $\delta_{\text{CP}}$ ,  $\alpha_{21}$  and  $\alpha_{31}$  with these relations by taking account of

$$\begin{aligned}
 \cos\delta_{\text{CP}} &= \frac{|U_{\tau 1}|^2 - s_{12}^2s_{23}^2 - c_{12}^2c_{23}^2s_{13}^2}{2c_{12}s_{12}c_{23}s_{23}s_{13}}, \\
 \text{Re} [U_{e1}^*U_{e2}] &= c_{12}s_{12}c_{13}^2 \cos\left(\frac{\alpha_{21}}{2}\right), \quad \text{Re} [U_{e1}^*U_{e3}] = c_{12}s_{13}c_{13} \cos\left(\frac{\alpha_{31}}{2} - \delta_{\text{CP}}\right). \quad (\text{D.4})
 \end{aligned}$$

In terms of this parametrization, the effective mass for the  $0\nu\beta\beta$  decay is given as follows:

$$\langle m_{ee} \rangle = \left| m_1c_{12}^2c_{13}^2 + m_2s_{12}^2c_{13}^2e^{i\alpha_{21}} + m_3s_{13}^2e^{i(\alpha_{31}-2\delta_{\text{CP}})} \right|. \quad (\text{D.5})$$

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