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Symplectic modular symmetry in heterotic string vacua: flavor, CP, and R -symmetries

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ABSTRACT: We examine a common origin of four-dimensional flavor, CP, and $U(1)_R$ symmetries in the context of heterotic string theory with standard embedding. We find that flavor and $U(1)_R$ symmetries are unified into the $Sp(2h+2, \mathbb{C})$ modular symmetries of Calabi-Yau threefolds with h being the number of moduli fields. Together with the $\mathbb{Z}_2^{\text{CP}}$ CP symmetry, they are enhanced to $GSp(2h+2, \mathbb{C}) \simeq Sp(2h+2, \mathbb{C}) \rtimes \mathbb{Z}_2^{\text{CP}}$ generalized symplectic modular symmetry. We exemplify the S_3, S_4, T', S_9 non-Abelian flavor symmetries on explicit toroidal orbifolds with and without resolutions and $\mathbb{Z}_2, S_4$ flavor symmetries on three-parameter examples of Calabi-Yau threefolds. Thus, non-trivial flavor symmetries appear in not only the exact orbifold limit but also a certain class of Calabi-Yau threefolds. These flavor symmetries are further enlarged to non-Abelian discrete groups by the CP symmetry.

KEYWORDS: Discrete Symmetries, Compactification and String Models, Superstrings and Heterotic Strings

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1 Introduction

The origin of flavor and CP symmetries is one of the unsolved and fundamental issues in the Standard Model. Understanding the underlying structure would give us a clue to find out the ultra-violet completion of the Standard Model. It was proposed in the pioneering works [1–11] that these symmetries are closely connected with the geometrical symmetry of extra-dimensional spaces. In particular, $SL(2, \mathbb{Z})$ modular symmetry is of particular interest in the bottom-up approach because the non-Abelian discrete flavor symmetries, which are used to explain flavor structure of quarks and leptons such as A_4 , S_4 , A_5 in the past decades, are naturally embedded into the $SL(2, \mathbb{Z})$, called the modular flavor symmetry [12]. The inclusion of the CP symmetry enlarges $SL(2, \mathbb{Z})$ to the generalized modular group $GL(2, \mathbb{Z})$ [13, 14].

From the viewpoint of top-down approach such as the string theory, the $SL(2, \mathbb{Z})$ symmetry appears in the low-energy effective action from the higher-dimensional theories on toroidal backgrounds [15, 16].¹ Furthermore, the flavor symmetry can be a quotient of $SL(2, \mathbb{Z})$, and CP symmetry can be regarded as an outer automorphism of $SL(2, \mathbb{Z})$. They can be treated in a unified manner [20]. The stabilization mechanism of moduli values providing observed masses and mixing angles of quarks/leptons is proposed in the context

¹Also, the modular symmetry, in particular, its anomaly was studied in refs. [17–19].

of string theory [21–23]. Hence, both flavor and CP symmetries have a common origin in the geometrical symmetries of toroidal backgrounds, and this approach would be useful to reveal the nature of extra-dimensional spaces relevant to particle physics.

In this paper, we examine the existence of modular flavor symmetry on Calabi-Yau (CY) threefolds which are promising backgrounds of the string theory. The complex structure and Kähler moduli spaces of CY threefolds are described by the symplectic structure with $\mathrm{Sp}(2h+2, \mathbb{Z})$ symplectic groups.² Here, h is determined by the number of the complex structure moduli $h = h^{2,1}$ or the Kähler moduli $h = h^{1,1}$. Such a symplectic extension was recently discussed in refs. [23, 26–28] in both bottom-up and top-down approaches, and these flavor symmetries are called the symplectic modular flavor symmetries. Since moduli fields and matter fields are in one-to-one correspondence with each other in the context of heterotic string theory with standard embedding, the flavor symmetries of matter fields naturally lie in symplectic modular flavor symmetries. In particular, it turned out that four-dimensional (4D) CP symmetry was regarded as the outer automorphism of $\mathrm{Sp}(2h+2, \mathbb{Z})$ on CY backgrounds [23]. These observations motivate us to examine the symplectic modular symmetry involving the flavor and CP symmetries in the context of CY symplectic moduli spaces.

The purpose of this paper is to formulate the symplectic modular flavor symmetries together with CP symmetry in the context of heterotic string theory with standard embedding and exemplify these symmetries on several toroidal and CY backgrounds. As discussed in detail in section 2, the flavor symmetries of fundamental and anti-fundamental representations of E_6 gauge group are governed by the symplectic modular symmetries in a general class of CY threefolds with large volume/complex structure, although the flavor structure depends on the intersection number of CY threefolds. Together with the results of ref. [23], we find that symplectic modular flavor symmetries are further enlarged to $G\mathrm{Sp}(2h+2, \mathbb{Z}) \simeq \mathrm{Sp}(2h+2, \mathbb{Z}) \rtimes \mathbb{Z}_2^{\mathrm{CP}}$, called “generalized symplectic modular symmetry”. Furthermore, the rotation of holomorphic three-form of CY threefolds induces that of Killing spinors of 4D supersymmetry, namely the $U(1)_R$ symmetry [29]. As a result, the flavor and the $U(1)_R$ symmetries are described by $\mathrm{Sp}(2h+2, \mathbb{C})$ symplectic modular symmetry, which results in the unification of all flavor, CP, and $U(1)_R$ symmetries in the context of $G\mathrm{Sp}(2h+2, \mathbb{C})$ symmetry. We explicitly demonstrate generalized symplectic modular symmetries on toroidal orbifolds with/without resolutions and three-parameter examples of CY threefolds. It turns out that there exist $G_{\mathrm{flavor}} = \mathbb{Z}_2, S_3, S_4, T', S_9$ non-Abelian flavor symmetries, and they are further enhanced into $G_{\mathrm{flavor}} \rtimes \mathbb{Z}_2^{\mathrm{CP}}$ together with the CP symmetry. So far, several techniques have been developed to understand G_{flavor} on toroidal orbifolds, but our approach is useful to find out the flavor structure of smooth CY threefolds, including the known toroidal orbifold regime. Indeed, our results indicate that a certain class of CY threefolds has the S_4 flavor symmetry on matter fields associated with the moduli fields.

This paper is organized as follows. In section 2, we briefly review the symplectic structure of moduli fields in CY compactifications and propose the generalized symplectic

²We refer the details about the symplectic modular symmetry to refs. [24, 25].

modular symmetries of matter fields in the context of heterotic string theory with standard embedding, where fundamental and anti-fundamental representations of E_6 group are directly related to Kähler moduli and complex structure moduli, respectively. The symplectic modular flavor symmetries and their enlarged symmetries by the CP transformation are explicitly demonstrated in section 3. Section 4 is devoted to conclusions and discussions. In appendix A, we give the modular form of weight 1 for T' .

2 Generalized symplectic modular symmetry

In section 2.1, we review the symplectic structure of moduli fields in CY compactifications with an emphasis on the large volume/complex structure regime. In section 2.2, we give a prescription of the symplectic modular flavor symmetry of matter fields associated with the complex structure moduli and Kähler moduli in the context of heterotic string theory with standard embedding. Furthermore, the symplectic transformations of matter fields naturally incorporate the existence of $U(1)_R$ symmetry appearing in the 4D effective action as shown in section 2.3. The CP transformations exchanging the fundamental and anti-fundamental representations of E_6 are regarded as the anti-holomorphic transformations of moduli fields. In section 2.4, we find that these anti-holomorphic transformations enlarge the symplectic modular symmetry into the generalized symplectic modular symmetry. As a result, the symplectic modular, flavor, CP, and $U(1)_R$ symmetries are treated in a unified manner.

2.1 Symplectic structure of moduli fields in Calabi-Yau compactifications

It was well known that the CY compactifications lead to the symplectic structure in the 4D effective action. (For more details about the symplectic structure of CY moduli spaces, see, e.g., refs. [24, 25].) The moduli fields associated with the CY metric are categorized into two types of moduli fields, i.e., the complex structure moduli and the Kähler moduli. Their Kähler potentials in the units of the reduced Planck mass are given by

$$\begin{aligned} K_{\text{cs}} &= -\ln \left[-i \int_{\mathcal{M}} \Omega \wedge \bar{\Omega} \right], \\ K_{\text{ks}} &= -\ln \left[\int_{\mathcal{M}} J_c \wedge J_c \wedge J_c \right], \end{aligned} \quad (2.1)$$

where Ω and J_c denote the holomorphic three-form and (complexified) Kähler form of CY threefolds $\mathcal{M}$, respectively. Here, $J_c = B + iJ$ consists of real Kalb-Ramond two-form B and Kähler form J . Their moduli spaces possess the symplectic structure. For concreteness, we will focus on the complex structure moduli with large complex structure, paying attention to the symplectic transformations of the moduli fields and the prepotential in subsequent discussions. The purpose of reviewing the symplectic structure is to understand the flavor structure of matter fields in the context of heterotic string theory with standard embedding, as will be discussed in the next section.

The holomorphic three-form Ω is expanded on the symplectic basis (α_I, β^I) of $H^3(\mathcal{M}, \mathbb{Z})$,³

$$\Omega = \sum_{I=0}^{h^{2,1}} \left(X^I \alpha_I - \mathcal{F}_I \beta^I \right), \quad (2.2)$$

where X^I are projective coordinates and the structure of $\mathcal{F}_I = \partial_I \mathcal{F}$ is determined by the prepotential $\mathcal{F}$. The orthogonal relation of the symplectic basis (α_I, β^I)

$$\int_{\mathcal{M}} \alpha_I \wedge \beta^J = \delta^J_I, \quad \int_{\mathcal{M}} \beta^J \wedge \alpha_I = -\delta^J_I, \quad (2.3)$$

is invariant under the symplectic transformation:

$$\begin{pmatrix} \alpha_I \\ \beta^I \end{pmatrix} \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \alpha_I \\ \beta^I \end{pmatrix}, \quad (2.4)$$

with

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{Sp}(2h^{2,1} + 2, \mathbb{Z}). \quad (2.5)$$

Correspondingly, the vector $\{X^I, \mathcal{F}_I\}^T$ (the so-called period integrals of holomorphic three-form)

$$\Pi = \begin{pmatrix} \int_{A^I} \Omega \\ \int_{B_I} \Omega \end{pmatrix} = \begin{pmatrix} X^I \\ \mathcal{F}_I \end{pmatrix} \quad (2.6)$$

transforms as

$$\begin{pmatrix} X^I \\ \mathcal{F}_I \end{pmatrix} \rightarrow \begin{pmatrix} \tilde{X}^I \\ \tilde{\mathcal{F}}_I \end{pmatrix} = \begin{pmatrix} d & c \\ b & a \end{pmatrix} \begin{pmatrix} X^I \\ \mathcal{F}_I \end{pmatrix}, \quad (2.7)$$

due to the fact that the holomorphic three-form is invariant under the symplectic transformation. Here, $\tilde{\mathcal{F}}_I$ is required to be a derivative of new function $\tilde{\mathcal{F}}(\tilde{X})$, namely $\tilde{\mathcal{F}}_I = \partial \tilde{\mathcal{F}}(\tilde{X}) / \partial \tilde{X}^I$, to remain within the same class of 4D effective action. Note that the 4D $\mathcal{N} = 2$ supersymmetric action is invariant under the symplectic transformation of the prepotential, $\tilde{\mathcal{F}}(\tilde{X}) = \mathcal{F}(X)$. Furthermore, when

$$\tilde{\mathcal{F}}(\tilde{X}) = \mathcal{F}(\tilde{X}), \quad (2.8)$$

the Lagrangian of $\mathcal{N} = 2$ supergravity with n Abelian vector multiplets is invariant under the symplectic transformations [30], although the prepotential itself is not invariant under them [31]. This structure holds for the system of our interest, i.e., string compactifications on $(2, 2)$ superconformal field theories [32–35].

³Note that the $\text{Sp}(2h^{2,1} + 2, \mathbb{C})$ appears in the classical moduli space, but loop and quantum corrections break it to $\text{Sp}(2h^{2,1} + 2, \mathbb{Z})$, namely duality transformations of the string theory.

From the symplectic transformation (2.7), it is found that $\{X^I\}$ takes a vector-valued modular form of $\mathrm{Sp}(2h^{2,1} + 2, \mathbb{Z})$, namely

$$X^I \rightarrow \tilde{X}^I = (c\mathcal{F} + d)_J^I X^J = \frac{\partial \tilde{X}^I}{\partial X^J} X^J, \quad (2.9)$$

and the symmetric tensor $\mathcal{F}_{IJK} = \partial_I \partial_J \partial_K \mathcal{F}$ obeys

$$\mathcal{F}_{IJK} \rightarrow \tilde{\mathcal{F}}_{IJK} = \frac{\partial X^L}{\partial \tilde{X}^I} \frac{\partial X^M}{\partial \tilde{X}^J} \frac{\partial X^N}{\partial \tilde{X}^K} \mathcal{F}_{LMN}, \quad (2.10)$$

where it is required that $\partial \tilde{X}^I / \partial X^J$ is a non-singular matrix. For instance, the invertible relation between $\tilde{X}^I$ and X^I is lost when the prepotential is a linear function of X^I as pointed out in ref. [31]. This formula is useful to understand the symplectic transformation of Yukawa couplings among matter fields as analyzed in detail below.

In the large complex structure regime,⁴ the prepotential is of the explicit form

$$\mathcal{F}(X) = \frac{1}{3!} \kappa_{ijk} \frac{X^i X^j X^k}{X^0} = (X^0)^2 F(u), \quad (2.11)$$

where κ_{ijk} denote the triple intersection numbers and the complex structure moduli u^i are set by

$$u^i \equiv \frac{X^i}{X^0}. \quad (2.12)$$

Here and in what follows, we still call $F(u) = \frac{1}{3!} \kappa_{ijk} u^i u^j u^k$ the prepotential and take the flat coordinates

$$X^0 = 1, \quad X^i = u^i. \quad (2.13)$$

Then, the symplectic transformation of the complex structure moduli u^i is given by

$$u^i \equiv X^i \rightarrow \tilde{u}^i = \frac{\tilde{X}^i}{\tilde{X}^0} = \frac{\partial \tilde{X}^i}{\partial X^J} \frac{X^J}{\tilde{X}^0} = \frac{\partial \tilde{X}^i}{\partial X^J} \frac{X^J}{\tilde{X}^0} = \frac{\partial \tilde{X}^i}{\partial X^J} \frac{u^J}{\tilde{X}^0} = (c\mathcal{F} + d)_J^i \frac{u^J}{\tilde{X}^0}. \quad (2.14)$$

Let us discuss the symplectic transformation of Yukawa couplings (F_{ijk}) among complex structure moduli. They are determined by the triple intersection numbers κ_{ijk} ,

$$F_{ijk} \equiv \frac{\partial}{\partial u^i} \frac{\partial}{\partial u^j} \frac{\partial}{\partial u^k} F(u) = X^0 \mathcal{F}_{ijk}(X) = \kappa_{ijk}, \quad (2.15)$$

which correspond to the holomorphic Yukawa couplings of matter fields in the context of heterotic string theory with standard embedding. The symplectic transformation of Yukawa couplings F_{ijk} can be read off from eq. (2.10), i.e.,

$$\tilde{F}_{ijk} = \frac{\partial}{\partial \tilde{u}^i} \frac{\partial}{\partial \tilde{u}^j} \frac{\partial}{\partial \tilde{u}^k} \tilde{F}(\tilde{u}) = \frac{\partial u^l}{\partial \tilde{u}^i} \frac{\partial u^m}{\partial \tilde{u}^j} \frac{\partial u^n}{\partial \tilde{u}^k} F_{lmn}, \quad (2.16)$$

⁴Throughout this paper, we analyze the classical CY moduli space.

or

$$\tilde{F}_{ijk} = \tilde{X}^0 \tilde{\mathcal{F}}_{ijk} = \tilde{X}^0 \frac{\partial X^L}{\partial \tilde{X}^i} \frac{\partial X^M}{\partial \tilde{X}^j} \frac{\partial X^N}{\partial \tilde{X}^k} \mathcal{F}_{LMN} = \tilde{X}^0 \frac{\partial X^l}{\partial \tilde{X}^i} \frac{\partial X^m}{\partial \tilde{X}^j} \frac{\partial X^n}{\partial \tilde{X}^k} F_{lmn}. \quad (2.17)$$

Hence, these two expressions lead to

$$\frac{\partial u^l}{\partial \tilde{u}^i} = (\tilde{X}^0)^{1/3} \frac{\partial X^l}{\partial \tilde{X}^i}. \quad (2.18)$$

So far, we have focused on the symplectic structure of the complex structure moduli space, but the same structure appears in the Kähler moduli space as discussed in detail in ref. [25]. When we introduce a basis of $H^2(\mathcal{M}, \mathbb{Z})$ as e_a , the Kähler moduli t^a are defined by

$$t^a e_a = B + iJ = J_c, \quad (2.19)$$

whose prepotential in the large volume regime is given by

$$\mathcal{G}(Y) = \frac{1}{3!} \kappa_{abc} \frac{Y^a Y^b Y^c}{Y^0} = (Y^0)^2 G(t), \quad (2.20)$$

with

$$t^a = \frac{Y^a}{Y^0}. \quad (2.21)$$

Here, κ_{abc} denote the triple intersection numbers among two cycles of CY threefolds, and $\{Y^A\}$ represent the projective coordinates on the Kähler moduli space. In particular, Y^0 is identified with the inverse of the axio-dilaton. Analogous to the complex structure moduli, the Kähler potential (2.1) is written by

$$\begin{aligned} K_{\text{cs}} &= -\ln \left[-i \int_{\mathcal{M}} \Omega \wedge \bar{\Omega} \right] = -\ln \left[-i (\bar{X}^I \mathcal{F}_I - X^I \bar{\mathcal{F}}_I) \right], \\ K_{\text{ks}} &= -\ln \left[\int_{\mathcal{M}} J_c \wedge J_c \wedge J_c \right] = -\ln \left[-i (\bar{Y}^A \mathcal{G}_A - Y^A \bar{\mathcal{G}}_A) \right], \end{aligned} \quad (2.22)$$

with $I = 0, 1, \dots, h^{2,1}$, $A = 0, 1, \dots, h^{1,1}$, and one can deal with the symplectic structure as summarized in table 1.

In the subsequent sections, we discuss the symplectic modular transformations of matter fields associated with the complex structure moduli and Kähler moduli. The flavor structure of matter fields can be read off from the symplectic structure of moduli Yukawa couplings.

2.2 Symplectic modular flavor symmetry of matter fields

In general, it is difficult to derive the flavor structure of matter fields in smooth CY compactifications due to the lack of analytical expression of the CY metric. Hence, we concentrate on the heterotic string theory with standard embedding to overcome this problem. The matter fields 27_a and $\bar{27}_i$ under the E_6 gauge group are in one-to-one correspondence with the Kähler moduli and the complex structure moduli, respectively. It indicates that

	Complex structure	Kähler structure
Projective coordinates	X^I $(I = 1, 2, \dots, h^{2,1} + 1)$	Y^A $(A = 1, 2, \dots, h^{1,1} + 1)$
Moduli fields	u^i $(i = 1, 2, \dots, h^{2,1})$	t^a $(a = 1, 2, \dots, h^{1,1})$
Prepotential	$\mathcal{F}(X) = (X^0)^2 F(u)$	$\mathcal{G}(Y) = (Y^0)^2 G(t)$
Kähler potential	$-\ln[-i(\bar{X}^I \mathcal{F}_I - X^I \bar{\mathcal{F}}_I)]$	$-\ln[-i(\bar{Y}^A \mathcal{G}_A - Y^A \bar{\mathcal{G}}_A)]$
Yukawa couplings	$\partial_i \partial_j \partial_k F = \kappa_{ijk}$	$\partial_a \partial_b \partial_c G = \kappa_{abc}$
Symplectic modular group	$\text{Sp}(2h^{2,1} + 2, \mathbb{Z})$	$\text{Sp}(2h^{1,1} + 2, \mathbb{Z})$
Symplectic transformations	$u^i \rightarrow (\tilde{X}^0)^{-1}(c\mathcal{F} + d)_j^i u^j$ $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{Sp}(2h^{2,1} + 2, \mathbb{Z})$	$t^a \rightarrow (\tilde{Y}^0)^{-1}(g\mathcal{G} + h)_b^a t^b$ $\begin{pmatrix} e & f \\ g & h \end{pmatrix} \in \text{Sp}(2h^{1,1} + 2, \mathbb{Z})$

Table 1. Moduli spaces of the complex structure and the Kähler structure.

the flavor structure of matter fields is directly related to the symplectic structure in the moduli spaces. In the following discussions, we assume that the matter zero-modes appear from either the complex structure moduli sector or the Kähler moduli sector since the net number of zero-modes is determined by

$$\chi = \frac{1}{2}|h^{2,1} - h^{1,1}|, \quad (2.23)$$

through the Atiyah-Singer index theorem. We will focus on the matter fields associated with either the complex structure moduli or the Kähler moduli in order to reveal the relation between the flavor symmetry of matter fields and symplectic modular symmetry appearing in the moduli effective action.

It was known that the matter Kähler metric is of the form⁵

$$\begin{aligned} K_{a\bar{b}}^{(27)} &= e^{\frac{1}{3}(K_{\text{cs}} - K_{\text{ks}})} (K_{\text{ks}})_{a\bar{b}}, \\ K_{i\bar{j}}^{(\overline{27})} &= e^{-\frac{1}{3}(K_{\text{cs}} - K_{\text{ks}})} (K_{\text{cs}})_{i\bar{j}}, \end{aligned} \quad (2.24)$$

where $(K_{\text{cs}})_{i\bar{j}} = \partial_i \partial_{\bar{j}} K_{\text{cs}}$, $(K_{\text{ks}})_{a\bar{b}} = \partial_a \partial_{\bar{b}} K_{\text{ks}}$, A^i and A^a denote the matter chiral superfields, respectively.⁶ At the moment, we study the relation between $\overline{27}_i$ matter fields and the complex structure moduli u^i for concreteness. The Kähler potential of the complex structure moduli in the large complex structure regime

$$K_{\text{cs}} = -\ln \left[-i \int_{\mathcal{M}} \Omega \wedge \bar{\Omega} \right] = -\ln \left[-i |X^0|^2 \frac{\kappa_{ijk}}{6} (u^i - \bar{u}^i)(u^j - \bar{u}^j)(u^k - \bar{u}^k) \right], \quad (2.25)$$

⁵The overall factor $e^{\pm \frac{1}{3}(K_{\text{cs}} - K_{\text{ks}})}$ takes the different form on toroidal orbifolds in the example of section 3 due to the enlarged symmetry [36].

⁶In the following, we call matter chiral superfields as matters for simplicity.

indicates that the matter Kähler metric obeys

$$K_{i\bar{j}}^{(\overline{27})} \propto |X^0|^{2/3} (K_{\text{cs}})_{i\bar{j}}, \quad (2.26)$$

up to the factor relevant to the Kähler moduli. Hence, symplectic transformations of $\overline{27}_i$ matter fields are almost the same with those of the moduli fields u^i , up to the X^0 factor. Indeed, the matter Kähler metric transforms under the symplectic modular transformations as

$$K_{i\bar{j}}^{(\overline{27})} \rightarrow |\tilde{X}^0|^{2/3} (K_{\text{cs}})_{\tilde{l}\tilde{m}} \frac{\partial \tilde{u}^i}{\partial u^l} \frac{\partial \tilde{u}^j}{\partial u^m} \quad (2.27)$$

up to the factor $e^{K_{\text{cs}}/3}$. It turns out that the Kähler potential of $\overline{27}_i$ matter fields has a modular invariance under the following symplectic transformation of matter fields:

$$A^i \rightarrow \tilde{A}^i = (\tilde{X}^0)^{1/3} \frac{\partial \tilde{u}^i}{\partial u^l} A^l = \frac{\partial \tilde{X}^i}{\partial X^j} A^j, \quad (2.28)$$

where we use eq. (2.18). Since the matrix

$$\frac{\partial \tilde{X}^i}{\partial X^j} = (c\mathcal{F} + d)_j^i \quad (2.29)$$

is an element of the subgroup of $\text{Sp}(2h^{2,1} + 2, \mathbb{Z})$, the flavor structure of matter fields is governed by the symplectic structure. In what follows, we adopt the gauge $X^0 = 1$ unless we specify it. As will be discussed later, the above modular transformation is indeed consistent with the Kähler invariance of the action by checking the Kähler invariant quantity.

On the other hand, the matter superpotential takes the form

$$W = F_{ijk} A^i A^j A^k, \quad (2.30)$$

where the matter Yukawa couplings are the same as the Yukawa couplings of the moduli fields. As we derived before, the $\text{Sp}(2h^{2,1} + 2, \mathbb{Z})$ modular transformations of their Yukawa couplings are provided by

$$\tilde{F}_{ijk} = \tilde{X}^0 \frac{\partial X^l}{\partial \tilde{X}^i} \frac{\partial X^m}{\partial \tilde{X}^j} \frac{\partial X^n}{\partial \tilde{X}^k} F_{lmn}. \quad (2.31)$$

Hence, we arrive at the symplectic modular transformation of the Kähler potential and the superpotential:

$$K_{\text{cs}} \rightarrow K_{\text{cs}} - \ln |\tilde{X}^0|^2, \quad W \rightarrow \tilde{X}^0 W, \quad (2.32)$$

from which the Kähler invariant quantity

$$e^K |W|^2 \quad (2.33)$$

is invariant under the symplectic modular transformation.

	$\overline{27}$ matter fields (Complex structure)	27 matter fields (Kähler structure)
Matter fields	A^i	A^a
Moduli fields	u^i	t^a
Superpotential	$F_{ijk} A^i A^j A^k$	$G_{abc} A^a A^b A^c$
Symplectic transformations	$A^i \rightarrow \tilde{A}^i = \frac{\partial \tilde{X}^i}{\partial X^j} A^j$	$A^a \rightarrow \tilde{A}^a = \frac{\partial \tilde{Y}^a}{\partial Y^b} A^b$
	$u^i \rightarrow \tilde{u}^i = (\tilde{X}^0)^{-1} \frac{\partial \tilde{X}^i}{\partial X^j} u^j$	$t^a \rightarrow \tilde{t}^a = (\tilde{Y}^0)^{-1} \frac{\partial \tilde{Y}^a}{\partial Y^b} t^b$
	$F_{ijk} \rightarrow \tilde{F}_{ijk} = \tilde{X}^0 \frac{\partial X^l}{\partial \tilde{X}^i} \frac{\partial X^m}{\partial \tilde{X}^j} \frac{\partial X^n}{\partial \tilde{X}^k} F_{lmn}$	$G_{abc} \rightarrow \tilde{G}_{abc} = \tilde{Y}^0 \frac{\partial Y^d}{\partial \tilde{Y}^a} \frac{\partial Y^e}{\partial \tilde{Y}^b} \frac{\partial Y^f}{\partial \tilde{Y}^c} G_{def}$
	$\frac{\partial \tilde{X}^i}{\partial \tilde{X}^j} = (c\mathcal{F} + d)_j^i$	$\frac{\partial \tilde{Y}^a}{\partial \tilde{Y}^b} = (g\mathcal{G} + h)_b^a$
Flavor symmetry	$G_{\text{flavor}} \subset \text{Sp}(2h^{2,1} + 2, \mathbb{Z})$	$G_{\text{flavor}} \subset \text{Sp}(2h^{1,1} + 2, \mathbb{Z})$

Table 2. Symplectic modular flavor symmetries.

We conclude that the flavor symmetry of matter fields $\overline{27}_i$, G_{flavor} , belongs to the $\text{Sp}(2h^{2,1} + 2, \mathbb{Z})$ modular symmetry,

$$G_{\text{flavor}} \subset \text{Sp}(2h^{2,1} + 2, \mathbb{Z}), \quad (2.34)$$

and the flavor structure is governed by the symplectic structure of the complex structure moduli. The same statements also hold for the 27_a matters associated with the Kähler moduli, whose prepotential is given in eq. (2.20) in the large volume regime. The flavor structure of 27_a matters is determined by the holomorphic Yukawa coupling κ_{abc} . For that reason, we call the flavor symmetry of matter fields the *symplectic modular flavor symmetry*. The symplectic transformations of matter zero-modes, moduli, and holomorphic Yukawa couplings are summarized in table 2. It is a natural generalization of $\text{Sp}(2, \mathbb{Z}) \simeq \text{SL}(2, \mathbb{Z})$ discussed in the toroidal background [1–11]. Since it is difficult to derive the flavor symmetries in a background-independent way, we explicitly demonstrate the existence of symplectic modular flavor symmetries on toroidal orbifolds with and without resolutions and some classes of CY threefolds in section 3.

2.3 $\text{U}(1)_R$ symmetry

In addition to the symplectic modular flavor symmetry, there exists a $\text{U}(1)_R$ symmetry in the 4D $\mathcal{N} = 1$ supersymmetric effective action. From the cubic matter superpotential (2.30), one can assign the R -charge $2/3$ for the matter fields in a conventional way due to the fact that the superpotential has R -charge 2. Here, we examine the $\overline{27}_i$ matter fields, but 27_a matter fields also have R -charge $2/3$ due to the same cubic superpotential. In this section, we discuss the relation between the symplectic modular symmetry and $\text{U}(1)_R$ symmetry.

Let us consider the symplectic transformations in the basis where the Yukawa couplings do not have the factor $\tilde{X}^0$,

$$\begin{aligned} A^i &\rightarrow \tilde{A}^i = (\tilde{X}^0)^{1/3} \frac{\partial \tilde{u}^i}{\partial u^l} A^l, \\ F_{ijk} &\rightarrow \tilde{F}_{ijk} = \frac{\partial u^l}{\partial \tilde{u}^i} \frac{\partial u^m}{\partial \tilde{u}^j} \frac{\partial u^n}{\partial \tilde{u}^k} F_{lmn}. \end{aligned} \quad (2.35)$$

Since the $U(1)_R$ symmetry is not the flavor symmetry, the $(\tilde{X}^0)^{1/3}$ factor appearing in the symplectic transformation of matter fields would play a role of R -symmetric transformation. In this respect, let us set

$$\tilde{X}^0 = e^{2i\alpha}, \quad (2.36)$$

with α being a constant relevant to the R -symmetric transformation [37]. This assignment is consistent with the symplectic modular symmetry and it gives rise to the R -charge 2 for the moduli fields. Indeed, the R -symmetric transformations for the period integrals in the large complex structure regime correspond to

$$\begin{pmatrix} X^I \\ \mathcal{F}_I \end{pmatrix} \rightarrow \begin{pmatrix} \tilde{X}^I \\ \tilde{\mathcal{F}}_I \end{pmatrix} = \tilde{X}^0 \begin{pmatrix} X^I \\ \mathcal{F}_I \end{pmatrix}, \quad (2.37)$$

with

$$\begin{aligned} \{X^0, X^i, \mathcal{F}_0, \mathcal{F}_i\} &= \left\{1, u^i, -\frac{1}{3!}\kappa_{ijk}u^i u^j u^k, \frac{1}{2}\kappa_{ijk}u^j u^k\right\}, \\ \{\tilde{X}^0, \tilde{X}^i, \tilde{\mathcal{F}}_0, \tilde{\mathcal{F}}_i\} &= \tilde{X}^0 \left\{1, \tilde{u}^i, -\frac{1}{3!}\kappa_{ijk}\tilde{u}^i \tilde{u}^j \tilde{u}^k, \frac{1}{2}\kappa_{ijk}\tilde{u}^j \tilde{u}^k\right\}. \end{aligned} \quad (2.38)$$

As stated in ref. [29], R -symmetric transformation corresponds to the holomorphic transformation f mapping the holomorphic three-form of CY threefolds Ω into a multiple of itself,

$$f \cdot \Omega = e^{i\gamma} \Omega, \quad (2.39)$$

with γ being the constant. Recalling that the Ω is constructed by a covariantly constant positive-chirality spinor η , namely $\Omega_{ijk} = \eta^T \Gamma_{ijk} \eta$ with three products of Gamma matrix Γ_{ijk} , the holomorphic mapping f rotates the η ,

$$f \cdot \eta = e^{i\gamma/2} \eta, \quad (2.40)$$

namely the 4D $\mathcal{N} = 1$ supersymmetry by a phase of $e^{i\gamma/2}$ for positive chirality spinor. The negative chirality spinor is rotated by an amount of $e^{-i\gamma/2}$. In this way, the phase shift of Ω gives rise to the R -symmetry in 4D $\mathcal{N} = 1$ supersymmetric theory. In our setup, our finding R -symmetric transformation $\tilde{X}^0 = e^{2i\alpha}$ corresponds to $\gamma = 2\alpha$. Note that the existence of $U(1)_R$ symmetry is related to the discrete $\mathbb{Z}_3^R$ R -symmetry appearing in the matter superpotential,

$$W = F_{ijk} A^i A^j A^k, \quad (2.41)$$

by assigning the charge 1 for all the matter fields. When we focus on the overall complex structure modulus $u^1 = u^2 = \dots = u^{h^{2,1}}$, the action is invariant under the overall $SL(2, \mathbb{Z})_{\text{overall}}$ symmetry. From the fact that the superpotential has modular weight -3 under $SL(2, \mathbb{Z})_{\text{overall}}$, the matter fields have charge -1. That would be related to the origin of charge 1 under the discrete $\mathbb{Z}_3^R$ R -symmetry.⁷ Similar statements also hold for the Kähler moduli space, by identifying Y^0 with the R -symmetric transformations of 27_a matter

⁷The relations between R -symmetry and the modular symmetry, in particular, their anomalies were studied in refs. [38, 39].

fields. Hence, R -symmetric transformations would be related to the phase rotation of the axio-dilaton. It is notable that the Kähler form consists of Killing spinors, $J_{m\bar{n}} = i\eta^\dagger \Gamma_{m\bar{n}} \eta$ with two products of Gamma matrix $\Gamma_{m\bar{n}}$ in the complex basis z^m with $m = 1, 2, 3$, but it does not change under the R -transformation.

As a result, $U(1)_R$ symmetry is also unified in the context of symplectic modular symmetry, i.e.,

$$\mathrm{Sp}(2h+2, \mathbb{C}) \supset \mathrm{Sp}(2h+2, \mathbb{Z}) \times U(1)_R, \quad (2.42)$$

with $h = h^{2,1}$ or $h^{1,1}$.

2.4 Unification of symplectic modular flavor, CP, and R -symmetries

Following refs. [40–42], one can identify the 4D CP symmetry with the simultaneous transformation of 4D parity and the 6D orientation reversing. They belong to the 10D proper Lorentz transformation. We recall that the 10D Majorana-Weyl spinor 16 decomposes under the 10D Lorentz symmetry $\mathrm{SO}(1, 9) = \mathrm{SO}(1, 3) \times \mathrm{SO}(6)$,

$$16 = (2_L, 4_+) \oplus (2_R, \bar{4}_-) \quad (2.43)$$

where 2_L and 2_R denote the left- and right-handed spinors of $\mathrm{SL}(2, \mathbb{C})$, and $4_+, \bar{4}_-$ represent the positive and negative chirality spinors of $\mathrm{SU}(4) \simeq \mathrm{SO}(6)$, respectively. Hence, the 4D parity and 6D orientation reversing exchanges $(2_L, 4_+)$ into $(2_R, \bar{4}_-)$ which is in one-to-one correspondence with the 4D CP transformation of E_6 matter fields: $27 \rightarrow \bar{27}$. It suggests that the 4D CP transformation is identified with the geometrical symmetry of the internal manifold.

The 6D orientation reversing changes the sign of the volume form of CY threefolds. In the local coordinate of CY threefolds z^m with $m = 1, 2, 3$, the following transformation

$$z^m \rightarrow -\bar{z}^m \quad (2.44)$$

changes the sign of the volume form.⁸ To see the orientation reversing of the volume form, we examine the transformation of the holomorphic three-form Ω and Kähler form J . Eq. (2.44) gives rise to the $\mathbb{Z}_2^{\mathrm{CP}}$ transformation:

$$\begin{aligned} \Omega &\rightarrow -\bar{\Omega}, \\ J_c &\rightarrow \bar{J}_c, \end{aligned} \quad (2.45)$$

where the anti-holomorphic transformation of Ω is consistent with its local expansion $\Omega = dz^1 \wedge dz^2 \wedge dz^3$. On CY threefolds, the 6D volume form dV is expressed by the Ω ,

$$i\Omega \wedge \bar{\Omega} = |\Omega|^2 dV, \quad (2.46)$$

thereby the transformation (2.45) changes the sign of the volume form, namely the 6D orientation reversing.

⁸The minus sign is a matter of convention.

We comment on the orientation reversing of the Kähler form J_c which is locally given by $J_c = B + iJ = (b_{m\bar{n}} + ig_{m\bar{n}})dz^m \wedge d\bar{z}^{\bar{n}}$, respectively. Recall that the real part of complexified Kähler form ($b_{m\bar{n}}$) originates from the Kalb-Ramond field, leading to the pseudo scalars (axions) in the 4D effective action through the hodge duality. Since the axions are 4D CP-odd fields through the 4D Chern-Simons couplings, $b_{m\bar{n}}$ is required to be transformed as $b_{m\bar{n}} \rightarrow -b_{m\bar{n}}$. By contrast, the imaginary part of complexified Kähler form ($g_{m\bar{n}}$) is a CP-even field. Hence, we arrive at the CP transformation of the complexified Kähler form as in eq. (2.45).

As discussed in ref. [43], the anti-holomorphic transformation of the holomorphic three-form induces the anti-holomorphic transformation of the complex structure moduli, and the CP-transformation of the complexified Kähler form also induces the anti-holomorphic transformation of the Kähler moduli due to the fact that $b_{m\bar{n}}$ and $g_{m\bar{n}}$ are CP-odd and -even fields, respectively. Then, we arrive at the CP transformation of the moduli fields:

$$u^i \rightarrow -\bar{u}^i, \quad t^a \rightarrow -\bar{t}^a, \quad (2.47)$$

where we take the convention with $\text{Im}(u^i) > 0$ and $\text{Im}(t^a) > 0$. Furthermore, since the real part of the axio-dilaton Y^0 originating from the Kalb-Ramond six-form is the universal axion, the CP transformation gives rise to

$$Y^0 \rightarrow -\bar{Y}^0. \quad (2.48)$$

It is trivial to check that these anti-holomorphic transformations are not the element of symplectic modular groups, but they belong to the generalized symplectic modular group $G\text{Sp}(2g + 2, \mathbb{Z}) \simeq \text{Sp}(2g + 2, \mathbb{Z}) \rtimes \mathbb{Z}_2^{\text{CP}}$ with $g = h^{2,1}, h^{1,1}$. Indeed, the $\mathbb{Z}_2^{\text{CP}}$ transformation acts on the projective coordinates in the complex structure and the Kähler structure moduli spaces⁹

$$\begin{pmatrix} X^0 \\ X^i \\ \mathcal{F}_0 \\ \mathcal{F}_i \end{pmatrix} \rightarrow - \begin{pmatrix} \bar{X}^0 \\ -\bar{X}^i \\ -\bar{\mathcal{F}}_0 \\ \bar{\mathcal{F}}_i \end{pmatrix} = \mathcal{CP} \begin{pmatrix} X^0 \\ X^i \\ \mathcal{F}_0 \\ \mathcal{F}_i \end{pmatrix}, \quad \begin{pmatrix} Y^0 \\ Y^a \\ \mathcal{G}_0 \\ \mathcal{G}_a \end{pmatrix} \rightarrow - \begin{pmatrix} \bar{Y}^0 \\ -\bar{Y}^a \\ -\bar{\mathcal{G}}_0 \\ \bar{\mathcal{G}}_a \end{pmatrix} = \mathcal{CP} \begin{pmatrix} Y^0 \\ Y^a \\ \mathcal{G}_0 \\ \mathcal{G}_a \end{pmatrix}, \quad (2.49)$$

with

$$\mathcal{CP} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \notin \text{Sp}(2h^{2,1} + 2, \mathbb{Z}), \text{Sp}(2h^{1,1} + 2, \mathbb{Z}). \quad (2.50)$$

Here, we use the shorthand notation for the identity matrix $\mathbf{1}$, which is rank $h^{2,1}$ for the complex structure moduli and $h^{1,1}$ for the Kähler moduli, respectively. Hence, they do not belong to the element of $\text{Sp}(2h^{2,1} + 2, \mathbb{Z})$ and $\text{Sp}(2h^{1,1} + 2, \mathbb{Z})$, due to the fact that the CP-transformation does not have the symplectic structure $\mathcal{CP}^T \cdot \Sigma \cdot \mathcal{CP} = \Sigma^T \neq \Sigma$. Rather, the CP transformation is regarded as an outer automorphism of the symplectic

⁹Here, we adopt the minus sign for the CP transformation in the complex structure moduli space, although the positive sign is allowed.

modular group, i.e., $\mathcal{CP} \cdot \gamma \cdot \mathcal{CP}^{-1}$ with γ being the transformation of the $\mathrm{Sp}(2h^{2,1} + 2, \mathbb{Z})$ or $\mathrm{Sp}(2h^{1,1} + 2, \mathbb{Z})$ modular group [23].¹⁰

As a result, the symplectic modular group together with the CP transformation is enlarged to the generalized symplectic modular group. In particular, the flavor symmetry belonging to the symplectic modular symmetry is also enhanced to the non-Abelian symmetry,

$$\begin{aligned} \mathrm{GSp}(2h^{2,1} + 2, \mathbb{Z}) &\supset G_{\mathrm{flavor}} \rtimes \mathbb{Z}_2^{\mathrm{CP}}, \\ \mathrm{GSp}(2h^{1,1} + 2, \mathbb{Z}) &\supset G_{\mathrm{flavor}} \rtimes \mathbb{Z}_2^{\mathrm{CP}}, \end{aligned} \quad (2.51)$$

as exemplified in the next section. The $\mathrm{U}(1)_R$ symmetry further enhances them into

$$\begin{aligned} \mathrm{GSp}(2h^{2,1} + 2, \mathbb{C}) &\supset G_{\mathrm{flavor}} \rtimes \mathbb{Z}_2^{\mathrm{CP}} \times \mathrm{U}(1)_R, \\ \mathrm{GSp}(2h^{1,1} + 2, \mathbb{C}) &\supset G_{\mathrm{flavor}} \rtimes \mathbb{Z}_2^{\mathrm{CP}} \times \mathrm{U}(1)_R. \end{aligned} \quad (2.52)$$

In the following analysis, we explicitly demonstrate the symplectic modular flavor symmetry on several backgrounds. This approach would be deserved to be the ultra-violet completion of the phenomenological model buildings in the bottom-up approach, where the symplectic modular flavor symmetry is used to explain the flavor structure of quarks and leptons.

3 Examples

In this section, we show the existence of generalized modular symmetry involving the flavor and CP symmetries on several backgrounds. Starting from the simplest 6D toroidal orbifolds in section 3.1, we deal with several blown-up toroidal orbifolds, where the size of blow-up radii is considered small enough in sections 3.2 and 3.3 and large enough in section 3.4. The three-parameter examples of CY threefolds are analyzed in section 3.5.

3.1 6D toroidal orbifolds

We begin with toroidal orbifolds with an emphasis on the flavor symmetry of untwisted modes. The twisted (blow-up) modes are analyzed in detail in the next sections. The simplest but non-trivial examples realizing the flavor symmetries of untwisted modes are based on $T^6/\mathbb{Z}_N$ and $T^6/(\mathbb{Z}_N \times \mathbb{Z}_M)$ with $h_{\mathrm{untw}}^{1,1} = 3$, whose prepotential is given by¹¹

$$G = t^1 t^2 t^3, \quad (3.1)$$

leading to the Kähler potential [36]

$$K_{\mathrm{ks}} = -\ln \left[i(t^1 - \bar{t}^1)(t^2 - \bar{t}^2)(t^3 - \bar{t}^3) - \sum_a |A^a|^2 \right] - \ln |Y^0|^2. \quad (3.2)$$

Here, we include Y^0 for the later purpose, and the matter fields are assumed to be expanded around $|A^a| \ll 1$. Correspondingly, the matter superpotential is of the form

$$W = Y^0 A^1 A^2 A^3. \quad (3.3)$$

¹⁰Outer automorphisms of flavor symmetries were studied as generalized CP symmetries [44–46].

¹¹The following discussions are applicable to the sector of $h^{2,1} = 3$ complex structure moduli sector as well.

Obviously, there appear the $\Pi_{a=1}^3 \text{SL}(2, \mathbb{Z})_a$ symmetries generated by

$$S^{(a)} : t^a \rightarrow -1/t^a, \quad T^{(a)} : t^a \rightarrow t^a + 1, \quad (3.4)$$

for $\Pi_{a=1}^3 \text{SL}(2, \mathbb{Z})_a$. They originate from factorizable three tori: $T^6 = (T^2)^3$. In addition, we find that there exists a S_4 symmetry by assigning $\{t^1, t^2, t^3\}$ for S_4 triplet and Y^0 for S_4 singlet. Although the S_4 group has two triplets $\{\mathbf{3}, \mathbf{3}'\}$ and two singlets $\{\mathbf{1}, \mathbf{1}'\}$, the superpotential is invariant under two cases: (i) $\{t^1, t^2, t^3\}$ for $\mathbf{3}$ and Y^0 for $\mathbf{1}$, (ii) $\{t^1, t^2, t^3\}$ for $\mathbf{3}'$ and Y^0 for $\mathbf{1}'$. (See for non-Abelian discrete symmetries and notation of representation, refs. [47, 48].) When we take the gauge $Y^0 = 1$, namely S_4 trivial singlet $\mathbf{1}$, the transformation of the S_4 triplet $\{t^1, t^2, t^3\}$ is given by

$$\begin{aligned} P : t^1 &\rightarrow t^3, & t^2 &\rightarrow t^1, & t^3 &\rightarrow t^2, \\ Q : t^1 &\rightarrow -t^1, & t^2 &\rightarrow -t^3, & t^3 &\rightarrow t^2, \end{aligned} \quad (3.5)$$

where P corresponds to S_3 permutation group of three $\text{SL}(2, \mathbb{Z})_a$ [49]. In the context of heterotic string theory with standard embedding, these symmetries are identified with the flavor symmetries of matter fields. Indeed, the matter fields $\{A^1, A^2, A^3\}$ are also identified with the S_4 triplet representation under which the effective action of matter fields is invariant.

Our purpose in this section is to check whether these symmetries together with the CP transformation can be embedded into the $G\text{Sp}(8, \mathbb{Z})$ generalized symplectic modular symmetry. The symplectic structure is understood from the symplectic transformation of the period vector

$$\begin{pmatrix} Y^A \\ \mathcal{G}_A \end{pmatrix} = \begin{pmatrix} Y^0 \\ Y^1 \\ Y^2 \\ Y^3 \\ \mathcal{G}_0 \\ \mathcal{G}_1 \\ \mathcal{G}_2 \\ \mathcal{G}_3 \end{pmatrix} = \begin{pmatrix} Y^0 \\ Y^1 \\ Y^2 \\ Y^3 \\ -Y^1 Y^2 Y^3 / (Y^0)^2 \\ Y^2 Y^3 / Y^0 \\ Y^1 Y^3 / Y^0 \\ Y^1 Y^2 / Y^0 \end{pmatrix} = Y^0 \begin{pmatrix} 1 \\ t^1 \\ t^2 \\ t^3 \\ -t^1 t^2 t^3 \\ t^2 t^3 \\ t^1 t^3 \\ t^1 t^2 \end{pmatrix}, \quad (3.6)$$

leading to the Kähler potential (3.2). Since the period vector is a fundamental representation of $\text{Sp}(8, \mathbb{Z})$, the symplectic transformation is represented by

$$\begin{pmatrix} Y^A \\ \mathcal{G}_A \end{pmatrix} = Y^0 \begin{pmatrix} 1 \\ t^1 \\ t^2 \\ t^3 \\ -t^1 t^2 t^3 \\ t^2 t^3 \\ t^1 t^3 \\ t^1 t^2 \end{pmatrix} \rightarrow \tilde{Y}^0 \begin{pmatrix} 1 \\ \tilde{t}^1 \\ \tilde{t}^2 \\ \tilde{t}^3 \\ -\tilde{t}^1 \tilde{t}^2 \tilde{t}^3 \\ \tilde{t}^2 \tilde{t}^3 \\ \tilde{t}^1 \tilde{t}^3 \\ \tilde{t}^1 \tilde{t}^2 \end{pmatrix} = Y^0 \times \mathcal{R} \begin{pmatrix} 1 \\ t^1 \\ t^2 \\ t^3 \\ -t^1 t^2 t^3 \\ t^2 t^3 \\ t^1 t^3 \\ t^1 t^2 \end{pmatrix}, \quad (3.7)$$

with $\mathcal{R} \subset \text{Sp}(8, \mathbb{Z})$.

It turns out that $\Pi_{a=1}^3 \text{SL}(2, \mathbb{Z})_a$ and S_4 symmetries are indeed subgroups of $\text{Sp}(8, \mathbb{Z})$. For instance, the generators of $\text{SL}(2, \mathbb{Z})_1$ and S_4 are chosen as¹²

$$\begin{aligned}
 S_1 &= \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, & T_1 &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \\
 P &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, & Q &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix},
 \end{aligned} \tag{3.8}$$

where the fundamental representation of $\text{Sp}(8, \mathbb{Z})$ is split into

$$\mathbf{8} = \mathbf{1} + \mathbf{3} + \mathbf{1} + \mathbf{3}, \tag{3.9}$$

under S_4 symmetry. We have focused on the transformation of moduli fields, but the S_4 flavor symmetry of matter fields is also realized by P and Q . Indeed, the submatrices of P and Q acting on $(t^1, t^2, t^3)^T$

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{3.10}$$

correspond to the transformations for untwisted matters $\{A^1, A^2, A^3\}$ with the S_4 triplet. Note that the holomorphic Yukawa coupling is invariant under this S_4 symmetry.

Let us discuss the origin of the S_4 symmetry in the effective action. We recall that imaginary parts of moduli $\text{Im}(t^a)$ behave as a triplet representation under $\text{SO}(3)$ group due to the fact that the volume form of factorizable toroidal background $\mathcal{V}$ is given by $\mathcal{V} \simeq \otimes_{a=1}^3 \text{Im}(t^a) dx^a \wedge dy^a$. Since the $\text{SO}(3)$ triplet representation corresponds to the S_4 triplet representation,¹³ S_4 symmetry exists in the moduli sector $\{\text{Im}(t^1), \text{Im}(t^2), \text{Im}(t^3)\}$. On the complexified Kähler form, the Kähler moduli consist of volume moduli $\text{Im}(t^a)$ and the Kähler axions $\text{Re}(t^a)$. This fact enhances $\text{SO}(3)$ into $\text{SU}(3)$ symmetry. On the other hand, matter fields are originated from 10D gauge bosons and gauginos. Since 10D $\mathcal{N} = 1$

¹²It is straightforward to obtain the generators of other $\text{SL}(2, \mathbb{Z})$ by flipping the corresponding moduli fields.

¹³See, e.g., ref. [50] and references therein.

supersymmetry gives rise to 4D $\mathcal{N} = 4$ supersymmetry equipping $SU(4)_R$ symmetry on T^6 background without orbifolding, the fundamental representation of $SU(4)_R$ symmetry can be split into

$$\mathbf{4} = \mathbf{1} + \mathbf{3}, \quad (3.11)$$

under the $SU(3)_R$ symmetry. The matter fields $\{A^a\}$ of our interest have triplet representation of $SU(3)_R$ symmetry, corresponding to the S_4 triplet representation. Indeed, the $SU(3)_R$ symmetry is embedded into $Sp(8, \mathbb{C})$ as follows:

$$R = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a_1 & a_2 & a_3 & 0 & 0 & 0 & 0 \\ 0 & a_4 & a_5 & a_6 & 0 & 0 & 0 & 0 \\ 0 & a_7 & a_8 & a_9 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a_1 & a_2 & a_3 \\ 0 & 0 & 0 & 0 & 0 & a_4 & a_5 & a_6 \\ 0 & 0 & 0 & 0 & 0 & a_7 & a_8 & a_9 \end{pmatrix}, \quad \text{with } \begin{pmatrix} a_1 & a_2 & a_3 \\ a_4 & a_5 & a_6 \\ a_7 & a_8 & a_9 \end{pmatrix} \in SU(3)_R, \quad (3.12)$$

where we used that $t^1 t^2 t^3 (A^1 A^2 A^3)$ is a $SU(3)_R$ singlet.

In this way, S_4 flavor symmetry naturally lies in the symplectic modular flavor symmetry. Together with the CP transformation as discussed in section 2.4, the symplectic modular symmetry is generalized to the generalized symplectic modular symmetry. It turns out that the S_4 flavor symmetry is enhanced to

$$S_4 \rtimes \mathbb{Z}_2^{\text{CP}}, \quad (3.13)$$

in a generic moduli space of $\{t^a\}$. Here, $\mathbb{Z}_2^{\text{CP}}$ transformation is given by eqs. (2.49) and (2.50).

3.2 Small resolutions of $T^6/\mathbb{Z}_3$ orbifold

In this section, we incorporate the twisted (blow-up) modes in the effective action on the 6D toroidal orbifolds. We mainly deal with the blown-up $T^6/\mathbb{Z}_3$ orbifold, which is directly connected with the effective action of untwisted modes in the previous section in the blow-down limit, i.e., the vanishing blow-up radii. On the blown-up $T^6/\mathbb{Z}_3$ geometry, only the Kähler structure deformations remain on the blown-up $T^6/\mathbb{Z}_3$ background. The totally $h^{1,1} = 36$ Kähler moduli include $h_{\text{untw}}^{1,1} = 9$ untwisted Kähler moduli and $h_{\text{tw}}^{1,1} = 27$ twisted Kähler moduli c^d ($d = 1, 2, \dots, 27$) from the viewpoint of toroidal orbifold.¹⁴ For simplicity, let us focus on the three diagonal untwisted Kähler moduli t^a ($a = 1, 2, 3$) whose moduli space is given by $\Pi_a SL(2, \mathbb{Z})_a$. The prepotential receives the corrections from the blow-up modes [36]

$$G = t^1 t^2 t^3 - \frac{i}{4} \sum_{d=1}^{27} (c^d)^2, \quad (3.14)$$

¹⁴The following discussion is applicable to the T-dual of $T^6/\mathbb{Z}_3$ orbifold, where the massless deformations correspond to the complex structure moduli accompanying the $\overline{27}_i$ matter fields. For more details, see, ref. [51] and references therein.

and the following vector

$$\begin{pmatrix} Y^A \\ \mathcal{G}_A \end{pmatrix} = \begin{pmatrix} 1 \\ t^1 \\ t^2 \\ t^3 \\ c^d \\ 2G - t^A \partial_A G \\ t^2 t^3 \\ t^1 t^3 \\ t^1 t^2 \\ -\frac{i}{2} c^d \end{pmatrix} = \begin{pmatrix} 1 \\ t^1 \\ t^2 \\ t^3 \\ c^d \\ -t^1 t^2 t^3 \\ t^2 t^3 \\ t^1 t^3 \\ t^1 t^2 \\ -\frac{i}{2} c^d \end{pmatrix}, \quad (3.15)$$

provides the Kähler potential

$$K_{\text{ks}} = -\ln \left[-i(\bar{Y}^A \mathcal{G}_A - Y^A \bar{\mathcal{G}}_A) \right] = -\ln \left[i(t^1 - \bar{t}^1)(t^2 - \bar{t}^2)(t^3 - \bar{t}^3) - \sum_d |c^d|^2 \right], \quad (3.16)$$

which is consistent with ref. [16]. Correspondingly, the matter Kähler metric is calculated through eq. (2.24).

The allowed Yukawa couplings of matter zero-modes are restricted by $\mathbb{Z}_3$ symmetry. The matter superpotential takes the form

$$W = A^1 A^2 A^3 - \sum_{d,e,f=1}^{27} f(t^1, t^2, t^3)_{def} C^d C^e C^f, \quad (3.17)$$

where C^d denotes the twisted matters associated twisted Kähler moduli, and their Yukawa couplings $f(t^1, t^2, t^3)_{def}$ are moduli-dependent in general [52–54]. The holomorphic Yukawa couplings of untwisted modes enjoy the S_4 flavor symmetry as previously discussed in the orbifold regime, but the flavor symmetry of the twisted matter fields is complicated. Before going into the detail of the Yukawa couplings among twisted matters, we comment on the S_4 symmetry of twisted matter fields. Let us denote them by fixed point labels, C_{n_1, n_2, n_3} , where $n_i = 0, 1, 2$ represents the fixed point label on the i -th $T^2/\mathbb{Z}_3$. The matter fields $C_{n,n,n}$ are obviously S_4 singlets. The other C_{n_1, n_2, n_3} are triplets because they transform each other under S_4 . Thus, 27 twisted matter fields decompose into three S_4 singlets and eight S_4 triplets.

In the blow-down limit treated in this section, the relevant modular symmetry in the untwisted Kähler moduli space is $\Pi_{a=1}^3 \text{SL}(2, \mathbb{Z})_a \subset \text{Sp}(8, \mathbb{Z})$. It was known that the Kähler metrics of untwisted and twisted matters take the form [18, 36]

$$\begin{aligned} K_{a\bar{b}}^{(27)}|_{\text{untw}} &= (K_{\text{ks}})_{a\bar{b}} e^{-K_a} = \frac{1}{i(t^a - \bar{t}^a)} \delta_{a\bar{b}}, \\ K_{d\bar{e}}^{(27)}|_{\text{tw}} &= (K_{\text{ks}})_{d\bar{e}} e^{-K_{\text{ks}}/3} = \frac{1}{\{i(t^1 - \bar{t}^1)(t^2 - \bar{t}^2)(t^3 - \bar{t}^3)\}^{2/3}} \delta_{d\bar{e}}, \end{aligned} \quad (3.18)$$

with $K_a = -\ln(-i(t^a - \bar{t}^a))$, from which we deduce the modular weight of both matter fields:

$$A^1 : \{-1, 0, 0\}, \quad A^2 : \{0, -1, 0\}, \quad A^3 : \{0, 0, -1\}, \quad C^d : \left\{-\frac{2}{3}, -\frac{2}{3}, -\frac{2}{3}\right\}, \quad (3.19)$$

under $\{\text{SL}(2, \mathbb{Z})_1, \text{SL}(2, \mathbb{Z})_2, \text{SL}(2, \mathbb{Z})_3\}$. These modular weights play an important role in checking the modular invariance of the action. Indeed, the matter superpotential of untwisted modes $A^1 A^2 A^3$ is invariant under the $\Pi_a \text{SL}(2, \mathbb{Z})_a$ modular symmetry due to its modular weight -1 under all $\text{SL}(2, \mathbb{Z})_a$. However, 3-point couplings of twisted modes $C^d C^e C^f$ have modular weight -2 under all $\text{SL}(2, \mathbb{Z})_a$. Hence, the modular invariance requires the moduli-dependent couplings $f(t^1, t^2, t^3)_{def}$ with modular weight 1 for each $\text{SL}(2, \mathbb{Z})_a$. It was known that the twisted modes belong to the triplet representation of double cover of $(A_4)_a$, namely $(T')_a \subset \text{SL}(2, \mathbb{Z})_a$ in the blow-down limit [16, 55], although this T' triplet is a reducible representation as seen below. Their holomorphic Yukawa couplings are expected to be a $\Gamma(3)$ modular form of non-Abelian discrete group A_4 , which bring into the $(T')_a$ -invariant superpotential. We will come back to this point later.

To see the T' structure in more detail, let us discuss T' transformations in the symplectic basis. Note that on this blown-up geometry, S_4 symmetry among untwisted modes lies in $\text{Sp}(8, \mathbb{Z}) \subset \text{Sp}(62, \mathbb{Z})$ in a way similar to the previous analysis. For concreteness, we focus on a subsector of twisted modes, i.e., three twisted fields $\{C^1, C^2, C^3\}$ which transform under the $\text{SL}(2, \mathbb{Z})_1$ symmetry. Then, the representations of these twisted matters under the S_1 and T_1 transformations of $\text{SL}(2, \mathbb{Z})_1$ are given by [16, 55]

$$\mathcal{S}_{\text{tw}} = -\frac{i}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & w & w^2 \\ 1 & w^2 & w \end{pmatrix}, \quad \mathcal{T}_{\text{tw}} = \begin{pmatrix} w & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (3.20)$$

with $w = e^{2\pi i/3}$. They satisfy the following algebraic relations:

$$\mathcal{S}_{\text{tw}}^2 = -\mathbb{I}, \quad (\mathcal{S}_{\text{tw}} \mathcal{T}_{\text{tw}})^3 = \mathcal{T}_{\text{tw}}^3 = \mathbb{I}, \quad (3.21)$$

which is the T' symmetry [47, 48]. Note that these matrices are rotated into

$$\mathcal{U}_{\text{tw}}^{-1} \mathcal{S}_{\text{tw}} \mathcal{U}_{\text{tw}} = -\frac{i}{\sqrt{3}} \begin{pmatrix} 1 & \sqrt{2} & 0 \\ \sqrt{2} & -1 & 0 \\ 0 & 0 & i \end{pmatrix}, \quad \mathcal{U}_{\text{tw}}^{-1} \mathcal{T}_{\text{tw}} \mathcal{U}_{\text{tw}} = \mathcal{T}_{\text{tw}}, \quad (3.22)$$

by the unitary transformation:

$$\mathcal{U}_{\text{tw}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \quad (3.23)$$

It indicates that T' triplet of our interest is a reducible representation decomposed into the singlet and the doublet representations.

We find that these transformations lie in the symplectic modular group as follows:

$$\begin{aligned}
 S_{\text{tw}} &= \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ & & & & \mathcal{S}_{\text{tw}} & & & \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ & & & & & & \mathcal{S}_{\text{tw}} & \end{pmatrix}, \\
 T_{\text{tw}} &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ & & & & \mathcal{T}_{\text{tw}} & & & \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ & & & & & & \mathcal{T}_{\text{tw}} & \end{pmatrix},
 \end{aligned} \tag{3.24}$$

where we omit 0 in the blank space for simplicity. Here, we focused on three twisted modes, but it is straightforward to extend this analysis on fully resolved toroidal orbifolds with small resolutions. In that case, the effective action enjoys the $(T')^3$ flavor symmetry belonging to $\text{Sp}(62, \mathbb{Z})$ modular symmetry.

Similar to the untwisted modes, T' flavor symmetry naturally lies in the symplectic modular flavor symmetry because it is a quotient of $\text{SL}(2, \mathbb{Z})$. The twisted modes have non-trivial representations under

$$(T')^3 \times S_4. \tag{3.25}$$

Thus, their vacuum expectation values may lead non-trivial breaking of $(T')^3 \times S_4$. Together with the CP transformation as discussed in section 2.4, symplectic modular symmetry is enlarged to the generalized symplectic modular symmetry. In the current setup, each T' flavor symmetry is enhanced to

$$T' \rtimes \mathbb{Z}_2^{\text{CP}} \simeq S_4, \tag{3.26}$$

as an element of $G\text{Sp}(62, \mathbb{Z})$. Note that $\mathbb{Z}_2^{\text{CP}}$ transformation exchanges between the irreducible representations of T' , i.e., the outer automorphism of T' .

To understand the nature of Yukawa couplings among twisted matters, we remind the couplings of twisted matters on $T^2/\mathbb{Z}_3$ geometry whose fixed points are labeled by $n = 0, 1, 2$. The total 27 fixed points on $T^6/\mathbb{Z}_3$ orbifold is reproduced by the product

of three fixed points on $T^2/\mathbb{Z}_3$. As a consequence of $\mathbb{Z}_3$ symmetry, Yukawa couplings of twisted modes localized on

$$(0, 0, 0), \quad (1, 1, 1), \quad (2, 2, 2), \quad (0, 1, 2) \quad (3.27)$$

are only allowed on $T^2/\mathbb{Z}_3$. In particular, their Yukawa couplings are of the form [52–54]

$$f(t^1, t^2, t^3)_{def} \propto e^{-\mathcal{A}}, \quad (3.28)$$

where $\mathcal{A}$ denotes the area satisfying boundary conditions relevant to twisted strings. Furthermore, these twisted strings wrap the cycle of toroidal orbifolds many times. Summing up these effects, the Yukawa couplings

$$f(t^1, t^2, t^3)_{def} \propto \sum_m e^{-\mathcal{A}_m} \quad (3.29)$$

will be elliptic functions such as theta functions as explicitly demonstrated on orbifolds. Note that the leading terms of holomorphic Yukawa couplings for (n, n, n) with $n = 0, 1, 2$ are constant, but the other one $(0, 1, 2)$ is exponentially suppressed with respect to the torus radii due to the fact that twisted strings propagate the fixed points with another. That is world-sheet instanton effects. The couplings among the fixed points $(0, 1, 2)$ would vanish if we neglect such world-sheet instanton effects.

Let us revisit these results in the context of symplectic modular symmetry, focusing on the modular transformation of Yukawa couplings on $T^2/\mathbb{Z}_3$. We denote the Yukawa coupling among three twisted modes on the same fixed point by Y_0 , while we denote the Yukawa couplings for three different fixed points $(0, 1, 2)$ and $(2, 1, 0)$ by Y_1 and Y_2 , following refs. [56, 57]. The triplet (Y_0, Y_1, Y_2) transforms in the same way as the three twisted modes, i.e., eq. (3.20), up to an overall phase. Thus, they decompose the singlet and doublet under T' , but the singlet corresponds to $(Y_1 - Y_2)$ and it vanishes automatically. The doublet corresponds to the modular forms of weight 1 for T' . Indeed, the modular forms of weight 1 for T' have two degrees of freedom, corresponding to the T' doublet [58]. Appendix A shows the modular form of weight 1 for T' in a representation basis.¹⁵ Indeed, this fact is well in accord with our observations. The constant Yukawa couplings localized at the fixed points (n, n, n) with $n = 0, 1, 2$ are the remnant of such modular functions in the large volume regime, whereas other one at $(0, 1, 2)$ are exponentially suppressed due to the structure of elliptic functions. The large volume expansion is nothing but the $q = e^{2\pi it}$ expansion in the modular form. So far, we have focused on $T^2/\mathbb{Z}_3$ orbifold, but the structure discussed above holds for the Yukawa couplings of twisted modes associated with 27 fixed points on $T^6/\mathbb{Z}_3$ orbifold.

In the limit that the values of blow-up moduli are sufficiently large, 27 twisted modes may have the flavor symmetry S_{27} in $\text{Sp}(54, \mathbb{Z})$ modular symmetry as the model in section 3.4. However, in the blow-down orbifold limit, the symmetry S_{27} as well as $\text{Sp}(54, \mathbb{Z})$ loses the geometrical meaning. However, twisted modes transform non-trivially under the

¹⁵Similar to twisted modes and their Yukawa couplings, zero-modes and their Yukawa couplings in magnetized D-brane models have non-trivial behavior under the modular symmetry [59–66].

$SL(2, \mathbb{Z})$ modular group of untwisted modes as the T' reducible triplet because of the structure of prepotential (3.14) and Kähler potential (3.16). That is a quite trivial transition of modular symmetric behavior of the twisted modes. However, we have understood just two regimes, i.e., sufficiently large blow-up moduli regime and the blow-down orbifold limit. The middle regime is unclear in our analysis. We hope to report on the whole picture of modular symmetric behavior in the future.

Finally, we comment on the other untwisted moduli whose moduli space is given by $\frac{SU(3,3)}{SU(3) \times SU(3) \times U(1)}$. From the prepotential of the untwisted modes

$$G = \sum_{a,b,c=1}^9 \kappa_{abc} t^a t^b t^c \quad (3.30)$$

with

$$\kappa_{123} = \kappa_{468} = \kappa_{579} = 1, \quad \kappa_{169} = \kappa_{258} = \kappa_{347} = -1, \quad (3.31)$$

and 0 otherwise, the Kähler potential of untwisted modes is provided by

$$K_{\text{ks}} = -\ln \left[-i \frac{\kappa_{abc}}{6} (t^a - \bar{t}^a)(t^b - \bar{t}^b)(t^c - \bar{t}^c) \right]. \quad (3.32)$$

Here, we take the $Y^0 = 1$ gauge. It is also known that the matter Kähler potential and corresponding metric are given by [67]

$$K = -\ln \det \left(-i(\mathcal{T} - \bar{\mathcal{T}}) - A_\alpha A_{\bar{\alpha}} \right)^{\hat{a}\hat{b}} = K_{\text{ks}} + (-i(\mathcal{T} - \bar{\mathcal{T}}))_{\hat{a}\hat{b}}^{-1} A_{\hat{a}}^{\hat{\alpha}} A_{\hat{b}}^{\hat{\beta}} + \mathcal{O}(|A|^4),$$

$$K_{\hat{a}\hat{b}}^{(27)} = (-i(\mathcal{T} - \bar{\mathcal{T}}))_{\hat{a}\hat{b}}^{-1}, \quad (3.33)$$

where

$$\mathcal{T} = \begin{pmatrix} t^1 & t^4 & t^5 \\ t^7 & t^2 & t^6 \\ t^8 & t^9 & t^3 \end{pmatrix}, \quad (3.34)$$

with $\hat{a}, \hat{b} = 1, 2, 3$. Note that α stands for the indices of $SU(3) \subset E_8$ gauge group which are different from the indices of $SU(3)$ isometry $\hat{a}$. The superpotential of untwisted modes is written by¹⁶

$$W = \sum_{\hat{a}, \hat{b}, \hat{c}, \alpha, \beta, \gamma} \kappa_{\hat{a}\hat{b}\hat{c}} \epsilon^{\alpha\beta\gamma} A_{\hat{a}}^{\hat{\alpha}} A_{\hat{b}}^{\hat{\beta}} A_{\hat{c}}^{\hat{\gamma}}, \quad (3.35)$$

with $\kappa_{\hat{1}\hat{2}\hat{3}} = 1$ and 0 otherwise, up to the overall factor, where $\epsilon^{\alpha\beta\gamma}$ are the anti-symmetric tensors of $SU(3) \subset E_8$ gauge group, and the upper and lower indices correspond to the $SU(3)$ isometry and $SU(3) \subset E_8$ gauge group, respectively. The S_4 flavor symmetry appears in three untwisted matters, e.g., $\{A_1^{\hat{1}}, A_1^{\hat{2}}, A_1^{\hat{3}}\}$ which can be embedded into the symplectic modular group following the previous procedures. In this way, the 9 untwisted modes transform as 3 triplet representations under the S_4 symmetry, that is, $\{A_{\hat{\alpha}}^{\hat{a}}, A_{\hat{\alpha}}^{\hat{b}}, A_{\hat{\alpha}}^{\hat{c}}\}$ for arbitrary α .

¹⁶The kinetic mixing of matter fields will play an important role of realizing the hierarchical structure of matter fields [68].

3.3 Small resolutions of $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ orbifold

We deal with another example to exemplify the existence of generalized symplectic modular symmetry. We focus on the small resolutions of $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ orbifold by further imposing $\mathbb{Z}'_3$ projection on $T^6/\mathbb{Z}_3$ orbifold. By introducing the complex coordinates of $\mathbb{C}^3$ as z^m , $m = 1, 2, 3$, we identify them with

$$z^m \simeq z^m + 1, \quad z^m \simeq z^m + \beta, \quad (3.36)$$

with $\beta = e^{2\pi i/6}$ to construct the three torus. Then, we specify the $\mathbb{Z}_3 \times \mathbb{Z}'_3$ action following ref. [43]:

$$\begin{aligned} \mathbb{Z}_3 : Q(z^m) &\simeq \beta^2 z^m, \\ \mathbb{Z}'_3 : Q'(z^m) &\simeq \beta^{2m} z^m + \frac{1+\beta}{3}, \end{aligned} \quad (3.37)$$

where $\mathbb{Z}'_3$ is a freely acting symmetry. From 27 fixed points under $\mathbb{Z}_3$ symmetry

$$z_{\text{fix}} = \frac{1+\beta}{3}(n_1, n_2, n_3), \quad (3.38)$$

with $n_m = 0, 1, 2$, we find 9 orbifold-invariant combinations:

$$\begin{aligned} f_1 : (0, 0, 0) + (1, 1, 1) + (2, 2, 2), & \quad f_2 : (0, 1, 2) + (1, 2, 0) + (2, 0, 1), \\ f_3 : (0, 2, 1) + (1, 0, 2) + (2, 1, 0), & \end{aligned} \quad (3.39)$$

$$\begin{aligned} f_4 : (1, 0, 0) + (2, 1, 1) + (0, 2, 2), & \quad f_5 : (0, 1, 0) + (1, 2, 1) + (2, 0, 2), \\ f_6 : (0, 0, 1) + (1, 1, 2) + (2, 2, 0), & \end{aligned} \quad (3.40)$$

$$\begin{aligned} f_7 : (2, 0, 0) + (0, 1, 1) + (1, 2, 2), & \quad f_8 : (0, 2, 0) + (1, 0, 1) + (2, 1, 2), \\ f_9 : (0, 0, 2) + (1, 1, 0) + (2, 2, 1). & \end{aligned} \quad (3.41)$$

Hence, there exist $h_{\text{tw}}^{1,1} = 9$ twisted Kähler moduli in addition to $h_{\text{untw}}^{1,1} = 3$ untwisted Kähler moduli.

The orbifold projection (3.37) breaks $(T')^3$ symmetry in section 3.2 to S_3 . For instance, eq. (3.39) represents the S_3 singlet, and eqs. (3.40) and (3.41) become S_3 triplets, although the triplet representation is the reducible representation decomposed into the single and doublet. In addition, 27 twisted modes on $T^6/\mathbb{Z}_3$ correspond to three singlets and eight triplets under the S_4 flavor symmetry of untwisted modes, where the matter fields $C_{n,n,n}$ correspond to the S_4 singlets, while the other C_{n_1, n_2, n_3} are S_4 triplets. All of the matter fields $C_{n,n,n}$ correspond to three fixed points in the linear combination f_1 . Here, the matter fields corresponding to both f_2 and f_3 become S_4 singlets because of the orbifold projection (3.37). On the other hand, the matter fields corresponding to (f_4, f_5, f_6) and (f_7, f_8, f_9) still represent the S_4 triplets. Thus, the orbifold projection (3.37) reduces three S_4 singlets and eight S_4 triplets to three S_4 singlets and two S_4 triplets. From the total $\text{Sp}(2 \times 12 + 2, \mathbb{Z})$ symplectic group, we can derive the S_3 flavor group,

$$\text{Sp}(26, \mathbb{Z}) \supset G_{\text{flavor}} = S_3, \quad (3.42)$$

where the embedding $S_3 \subset \text{Sp}(8, \mathbb{Z}) \subset \text{Sp}(26, \mathbb{Z})$ is realized by following the same step in the previous section. The S_3 generator corresponds to P in eq. (3.5). Then, the S_3 flavor symmetry is enlarged to $D_6 \simeq S_3 \rtimes \mathbb{Z}_2^{\text{CP}} \subset \text{GSp}(26, \mathbb{Z})$, taking into account the CP symmetry. Here, $\mathbb{Z}_2^{\text{CP}}$ transformation is given by eqs. (2.49) and (2.50).

In the following, we move to the geometrical regime where the size of blow-up radii is above the string length and check whether there exist such discrete modular flavor symmetries.

3.4 Geometrical regime of blown-up $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ orbifold

In the previous sections, we examined the blown-up toroidal orbifolds with small resolutions, where the S_3 , S_4 , and T' flavor symmetries among untwisted and twisted matters are independent. Together with the CP symmetry, all of them belong to the generalized symplectic modular symmetry and are enlarged to D_6 , $S_4 \rtimes \mathbb{Z}_2^{\text{CP}}$ and S_4 , respectively.

In contrast to the previous analysis assuming the small vacuum expectation values of blow-up modes, we discuss more non-trivial examples on smooth CY threefolds. In this section, we focus on $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ background, where the blown-up cycles are larger than 1 in string units, in comparison with the analysis of section 3.3. Among $h^{1,1} = 12$ Kähler moduli, there exist $h_{\text{untw}}^{1,1} = 3$ untwisted Kähler moduli spanned by e_a corresponding to $idz^a \wedge d\bar{z}^{\bar{b}}$ from the viewpoint of toroidal orbifold, where z^a ($a = 1, 2, 3$) denote the coordinates of 3-torus. In addition, we have $h_{\text{tw}}^{1,1} = 9$ twisted Kähler moduli spanned by e_r ($r = 1, 2, \dots, 9$), corresponding to complex projective spaces $\mathbb{P}^2$'s, where fixed points are now resolved as $\mathbb{P}^2$ of a $\mathbb{C}^3/\mathbb{Z}_3$ singularity. On this geometry, there is no complex structure deformation.

When we expand the Kähler form

$$J = \sum_{a=1}^3 t^a e_a + \sum_{r=1}^9 v^r e_r, \quad (3.43)$$

the Kähler potential is evaluated as [69]

$$K_{\text{KS}} = -\ln \int J_c \wedge J_c \wedge J_c = -\ln \frac{1}{8} \left[81(t^1 - \bar{t}^1)(t^2 - \bar{t}^2)(t^3 - \bar{t}^3) - \frac{3}{2} \sum_r (v^r - \bar{v}^r)^3 \right]. \quad (3.44)$$

Here, the prepotential is given by

$$G = \frac{\kappa_{ABC}}{6} t^A t^B t^C = 81 t^1 t^2 t^3 - \frac{3}{2} \sum_r (v^r)^3, \quad (3.45)$$

with the nonvanishing triple intersection numbers,

$$\kappa_{123} = 81, \quad \kappa_{rrr} = -9. \quad (3.46)$$

Hence, the corresponding matter superpotential takes the form

$$W = 81 A^1 A^2 A^3 - 9 \sum_{r=1}^9 (V^r)^3, \quad (3.47)$$

where $A^{1,2,3}$ and V^r denote the matter fields associated with the untwisted and twisted moduli fields from the viewpoint of toroidal orbifolds, respectively. The matter Kähler metric is calculated through eq. (2.24). We find that the matter superpotential is invariant under two flavor symmetries: S_4 symmetry for the untwisted matters $\{A^1, A^2, A^3\}$ and S_9 symmetry for the twisted matters $\{V^1, V^2, \dots, V^9\}$ in addition to the overall modular symmetry $\text{SL}(2, \mathbb{Z})_{\text{overall}}$.

To see the relation between flavor symmetries of matter fields and symplectic modular symmetry, let us consider the period vector providing the Kähler potential (3.44). Since the blown-up $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ manifold have totally 12 Kähler moduli fields, the moduli space is described by $\text{Sp}(26, \mathbb{Z})$ symplectic modular symmetry. Correspondingly, the period vector is given by

$$\begin{pmatrix} Y^A \\ \mathcal{G}_A \end{pmatrix} = \begin{pmatrix} 1 \\ t^1 \\ t^2 \\ t^3 \\ v^r \\ 2G - t^A \partial_A G \\ 81t^2 t^3 \\ 81t^1 t^3 \\ 81t^1 t^2 \\ -\frac{9}{2}(v^r)^2 \end{pmatrix} = \begin{pmatrix} 1 \\ t^1 \\ t^2 \\ t^3 \\ v^a \\ -81t^1 t^2 t^3 + \frac{3}{2} \sum_r (v^r)^3 \\ 81t^2 t^3 \\ 81t^1 t^3 \\ 81t^1 t^2 \\ -\frac{9}{2}(v^r)^2 \end{pmatrix}. \quad (3.48)$$

Similar to the previous example, the S_4 flavor symmetry of the untwisted moduli $\{t^1, t^2, t^3\}$ can be embedded into $\text{Sp}(8, \mathbb{Z}) \subset \text{Sp}(26, \mathbb{Z})$. Accordingly, the matter fields $A^{1,2,3}$ transform as in eq. (3.10). In addition, we find that the generators of S_9

$$\mathcal{P}_{rs} : v^r \leftrightarrow v^s \quad (3.49)$$

is the element of $\text{Sp}(26, \mathbb{Z})$ as follows. For an illustrative purpose, let us focus on $\mathcal{P}_{12}$ exchanging v^1 and v^2 . To shorten the expression of the generator $\mathcal{P}_{12}$, we focus on the relevant period vector transformed under $\mathcal{P}_{12}$,

$$\begin{pmatrix} v^1 \\ v^2 \\ -\frac{9}{2}(v^1)^2 \\ -\frac{9}{2}(v^2)^2 \end{pmatrix}, \quad (3.50)$$

on which $\mathcal{P}_{12}$ acts on

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} v^1 \\ v^2 \\ -\frac{9}{2}(v^1)^2 \\ -\frac{9}{2}(v^2)^2 \end{pmatrix} = \begin{pmatrix} v^2 \\ v^1 \\ -\frac{9}{2}(v^2)^2 \\ -\frac{9}{2}(v^1)^2 \end{pmatrix}. \quad (3.51)$$

$\mathcal{P}_{12}$ acts the identity operators on the other elements of period vector. In this way, we show that the generator $\mathcal{P}_{12}$ is the element of $\text{Sp}(26, \mathbb{Z})$, and it is possible to prove the other $\mathcal{P}_{rs}$ as the element of $\text{Sp}(26, \mathbb{Z})$ by changing the indices of $v^{r,s}$.

These transformations are directly related to the S_9 flavor symmetry of matter fields from $\mathcal{P}_{rs}$. Indeed, the submatrix of $\mathcal{P}_{rs}$ acting on $(v^1, v^2)^T$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (3.52)$$

corresponds to the transformation between V^1 and V^2 . Combining all $\mathcal{P}_{ab}$ acting on

$$(v^1, v^2, v^3, v^4, v^5, v^6, v^7, v^8, v^9)^T, \quad (3.53)$$

one can realize the transformations of matter fields under S_9 modular flavor symmetry.

We conclude that there exist $G_{\text{flavor}} = S_4 \times S_9$ flavor symmetries in the effective action of blown-up $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ orbifold. They originate from the $\text{Sp}(26, \mathbb{Z})$ symplectic group,

$$\text{Sp}(26, \mathbb{Z}) \supset G_{\text{flavor}} = S_4 \times S_9, \quad (3.54)$$

where S_9 symmetry is broken down to S_3 in the regime with small resolutions as in section 3.3. That would be related to the spontaneous breaking of flavor symmetry triggered by the blow-up modes. We will leave the more detailed discussion of this symmetry breaking involving the stabilization of blow-up modes to future work. When we take into account the CP transformation, two flavor symmetries are enhanced to

$$S_4 \rtimes \mathbb{Z}_2^{\text{CP}}, \quad S_9 \rtimes \mathbb{Z}_2^{\text{CP}}. \quad (3.55)$$

In the next section, we show the existence of non-Abelian discrete flavor symmetries on other classes of CY threefolds.

This example suggests that some class of models with h blow-up modes may lead to the superpotential

$$W = \sum_{i=1}^h (A^i)^3, \quad (3.56)$$

up to an overall factor. This superpotential seems to have the S_h flavor symmetry, which is the permutation among A^i . This type of superpotential has a specific property for $h = 3$. We start with the following superpotential:

$$W = \tilde{A}^1 \tilde{A}^2 \tilde{A}^3. \quad (3.57)$$

Here, we redefine the matter fields,

$$\begin{aligned} \tilde{A}^1 &= A^1 + A^2 + A^3, \\ \tilde{A}^2 &= A^1 + \omega A^2 + \omega^2 A^3, \\ \tilde{A}^3 &= A^1 + \omega^2 A^2 + \omega A^3. \end{aligned} \quad (3.58)$$

Then, we can write

$$W = \tilde{A}^1 \tilde{A}^2 \tilde{A}^3 = (A^1)^3 + (A^2)^2 + (A^3)^2. \quad (3.59)$$

The S_3 symmetry is enlarged to S_4 . Hence, this phenomenon can be observed only for $h = 3$.

3.5 Three-parameter examples of Calabi-Yau threefolds

So far, we have focused on the toroidal orbifolds with and without resolutions. In this section, we analyze the smooth CY threefolds, emphasizing the flavor symmetry of matter fields. In particular, we deal with the Kreuzer-Skarke data set of CY threefolds, given by total 473,800,776 ambient toric fourfolds [70]. The ambient toric varieties are described by the corresponding (reflexive) polytope, which might involve singularities in general. The smooth CY hypersurfaces are obtained through “triangulation” of the polytope where the singularities of the ambient space are resolved. For the favorable CY hypersurface X ,¹⁷ the harmonic (1,1)-forms for $H^2(X, \mathbb{Z})$, J_r with $r = 1, 2, \dots, h^{1,1}$, can be obtained by the pull-backs of (1,1)-forms on the ambient space. Then, the intersection numbers d_{rst} of X can be calculated by

$$d_{rst} = \int_X J_r \wedge J_s \wedge J_t. \quad (3.60)$$

Here, the J_r stand for the basis of the Picard group. Finally, we describe the Kähler cone of X , determining the allowed Kähler moduli t^r . For the favorable CY hypersurface, the Kähler cone of X is also derived from that of the ambient space whose Kähler cone is calculated by the data of polytope. When we expand the (1,1)-form J as $J = t^r J_r$, the Kähler moduli t^r satisfy

$$\sum_r K_r^{\hat{r}} t^r \geq 0, \quad (3.61)$$

where we introduce the Kähler cone matrix $K = [K_r^{\hat{r}}]$ and $\hat{r}$ runs over the facets of the Kähler cone. Note that the two examples we analyze later have a few different triangulation corresponding to a partial resolution for the ambient toric varieties. In that case, the Kähler cone is given by the union of several sub-cones:

$$K = \bigcup_j K_j. \quad (3.62)$$

Among them, only 16 manifolds have a non-trivial fundamental group which is an important ingredient in introducing Wilson-lines on quotient CY threefolds [71]. We focus on these particular class of CY threefolds in the context of heterotic string theory with standard embedding.¹⁸ For illustrative purposes, we deal with five quotient CY threefolds. (For more details about the toric data as well as topological data of CY threefolds, we refer to ref. [72].) In particular, we focus on the Kähler moduli sector by assuming that the complex structure moduli sector is stabilized by some mechanism at a high scale.

1. The first example of CY threefold with non-trivial fundamental group has $h^{1,1} = 3$ Kähler moduli, $h^{2,1} = 59$ complex structure moduli, i.e., Euler number $\chi = -112$ (corresponding to the “downstairs” CY threefold X_{14} in ref. [72]). We will focus on

¹⁷The favorable CY means that the hodge number $h^{1,1}$ of X is the same with that of the ambient space.

¹⁸The heterotic string models in the context of non-standard embedding are discussed on such a particular class of CY threefolds [72].

the Kähler moduli sector since the complex structure moduli sector is complicated to analyze. The prepotential in the Kähler moduli sector is given by

$$G = t^1 t^2 t^3, \quad (3.63)$$

with non-vanishing triple intersection number $\kappa_{123} = 1$. The Kähler cone is given by $K = \text{diag}(1, 1, 1)$. Hence, the superpotential of matter fields associated with the Kähler moduli has the same functional form as one in the example of section 3.2,

$$W = A^1 A^2 A^3. \quad (3.64)$$

Hence, in addition to $\Pi_{a=1}^3 \text{SL}(2, \mathbb{Z})_a$, there exists the S_4 flavor symmetry, which can be enhanced to $S_4 \rtimes \mathbb{Z}_2^{CP}$ symmetry, taking into account the CP transformation. The symmetry is then embedded into the generalized symplectic $\text{Sp}(8, \mathbb{Z})$ flavor symmetry in the Kähler moduli space.

2. The second example of three Kähler parameters of CY has $h^{2,1} = 59$ complex structure moduli, i.e., Euler number $\chi = -112$ (corresponding to the downstairs CY threefold X_6 in ref. [72]). When we focus on the Kähler moduli sector, the prepotential is given by

$$G = t^1 t^2 t^3 - 2t^2 (t^3)^2, \quad (3.65)$$

with non-vanishing triple intersection numbers $\kappa_{123} = 1$ and $\kappa_{233} = -4$. Here, the intersection number is negative, but it is possible to redefine the modulus field as $\tilde{t}^1 \equiv t^1 - 2t^3$, corresponding to the Kähler cone $K = \text{diag}(1, 1, 1)$. It provides the superpotential of matter fields associated with the Kähler moduli,

$$W = A^1 A^2 A^3 - 2A^2 (A^3)^2, \quad (3.66)$$

which has a flavor structure similar to the first example of CY. Indeed, when we redefine the matter fields as $\tilde{A}^1 \equiv A^1 - 2A^3$, the matter superpotential reduces to

$$W = \tilde{A}^1 A^2 A^3. \quad (3.67)$$

Hence, we find that S_4 flavor symmetry is realized on this class of CY threefold and its enhanced $S_4 \rtimes \mathbb{Z}_2^{CP}$ symmetry together with the CP transformation can be embedded into the generalized symplectic $\text{Sp}(8, \mathbb{Z})$ flavor symmetry.

3. The third example of three Kähler parameters of CY has $h^{2,1} = 43$ complex structure moduli, i.e., Euler number $\chi = -80$ (corresponding to the downstairs CY threefold X_5 in ref. [72]). The prepotential in the Kähler moduli sector is given by

$$G = t^1 t^2 t^3 - 2t^1 (t^3)^2 + 2t^2 (t^3)^2 - 8(t^3)^3, \quad (3.68)$$

with non-vanishing triple intersection numbers $\kappa_{123} = 1$, $\kappa_{133} = -4$, $\kappa_{233} = 4$ and $\kappa_{333} = -48$. Here, the Kähler cone is given by

$$K = \begin{pmatrix} 0 & 1 & -2 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (3.69)$$

constraining the Kähler moduli to satisfy eq. (3.61). It provides the superpotential of matter fields associated with the Kähler moduli,

$$W = A^1 A^2 A^3 - 2A^1 (A^3)^2 + 2A^2 (A^3)^2 - 8(A^3)^3. \quad (3.70)$$

There is the overall modular symmetry $\text{SL}(2, \mathbb{Z})_{\text{overall}}$. It seems that other non-trivial flavor symmetries are absent in this system. There is $\mathbb{Z}_2$ symmetry such as

$$A^1 \rightarrow A^2, \quad A^2 \rightarrow A^1, \quad A^3 \rightarrow -A^3, \quad (3.71)$$

up to $\text{U}(1)_R$ symmetry $W \rightarrow -W$.

4. The fourth example of three Kähler parameters of CY has $h^{2,1} = 75$ complex structure moduli, i.e., Euler number $\chi = -144$ (corresponding to the downstairs CY threefold X_7 in ref. [72]). The prepotential in the Kähler moduli sector is given by

$$G = t^1 t^2 t^3 - 2(t^2)^2 t^3 - 2t^1 (t^3)^2 + 8(t^3)^2, \quad (3.72)$$

with non-vanishing triple intersection numbers $\kappa_{123} = 1$, $\kappa_{223} = \kappa_{133} = -4$ and $\kappa_{333} = 48$. Here, the Kähler cone is given by

$$K = \begin{pmatrix} 1 & -2 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & -2 \end{pmatrix}, \quad (3.73)$$

constraining the Kähler moduli to satisfy eq. (3.61). It provides the superpotential of matter fields associated with the Kähler moduli,

$$W = A^1 A^2 A^3 - 2(A^2)^2 A^3 - 2A^1 (A^3)^2 + 8(A^3)^2. \quad (3.74)$$

There is the overall modular symmetry $\text{SL}(2, \mathbb{Z})_{\text{overall}}$, but other non-trivial flavor symmetries are absent in this system.

5. The last example of three Kähler parameters of CY has $h^{2,1} = 75$ complex structure moduli, i.e., Euler number $\chi = -144$ (corresponding to the downstairs CY threefold X_8 in ref. [72]). The prepotential in the Kähler moduli sector is given by

$$G = t^1 t^2 t^3 - 2t^1 (t^3)^2 - 2t^2 (t^3)^2 + 8(t^3)^2, \quad (3.75)$$

with non-vanishing triple intersection numbers $\kappa_{123} = 1$, $\kappa_{133} = \kappa_{233} = -4$ and $\kappa_{333} = 48$. Here, the Kähler cone is given by

$$K = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & -2 \\ 0 & 1 & -2 \end{pmatrix}, \quad (3.76)$$

constraining the Kähler moduli to satisfy eq. (3.61). It provides the superpotential of matter fields associated with the Kähler moduli,

$$W = A^1 A^2 A^3 - 2A^1 (A^3)^2 - 2A^2 (A^3)^2 + 8(A^3)^2. \quad (3.77)$$

There is the overall modular symmetry $\mathrm{SL}(2, \mathbb{Z})_{\text{overall}}$. In addition, there exists a $\mathbb{Z}_2 \simeq S_2$ flavor symmetry between A^1 and A^2 and it is further enhanced to $\mathbb{Z}_2 \rtimes \mathbb{Z}_2^{\mathrm{CP}}$ symmetry, taking into account the CP transformation. Since the $\mathbb{Z}_2$ transformation is the same with $\mathcal{P}_{12}$ in eq. (3.51), the symmetry is then embedded into the $\mathrm{Sp}(8, \mathbb{Z})$ generalized symplectic flavor symmetry.

We find that non-trivial flavor symmetries on three-parameter examples of CY threefolds are given by S_4 and $\mathbb{Z}_2$ symmetries, enlarging to $S_4 \rtimes \mathbb{Z}_2^{\mathrm{CP}}$ and $\mathbb{Z}_2 \rtimes \mathbb{Z}_2^{\mathrm{CP}}$ taking into account the $\mathbb{Z}_2^{\mathrm{CP}}$ symmetry. Hence, the S_4 flavor symmetry appears in not only the exact orbifold limit but also a certain class of CY threefolds such as the first and second examples. In addition, all examples enjoy the overall modular symmetry $\mathrm{SL}(2, \mathbb{Z})_{\text{overall}}$, which looks $\mathbb{Z}_3$ symmetry, $A^i \rightarrow e^{2\pi i/3} A^i$ in the field-theoretical viewpoint. The above S_4 and $\mathbb{Z}_2$ symmetries are commutable with this $\mathbb{Z}_3$ symmetry.

Our analysis is limited to specific CY threefolds, but it is interesting to examine the flavor symmetries on a more broad class of CY threefolds. We leave it for future work.

4 Conclusions and discussions

In this paper, we examined the origin of flavor symmetry in the context of heterotic string theory on CY threefolds, including toroidal orbifolds. The flavor structure of matter zero-modes in the context of heterotic string theory with standard embedding is governed by the geometrical structure of CY threefolds because the matter and moduli fields are in one-to-one correspondence with each other. It indicates that the flavor structure is closely related to the symplectic structure of CY moduli spaces. Furthermore, the 4D CP and the $\mathrm{U}(1)_R$ symmetries were regarded as the outer automorphism of the symplectic modular group [23] and the rotation of holomorphic three-form of CY threefolds [29], respectively. These observations motivate us to thoroughly investigate the relation among flavor, CP, and $\mathrm{U}(1)_R$ symmetries on the basis of 4D effective action. This approach would yield the ultra-violet origin of models with modular flavor symmetry in the bottom-up approach.

In section 2, we gave a unified picture of these flavor, CP, and $\mathrm{U}(1)_R$ symmetries from the viewpoint of generalized symplectic symmetry $G\mathrm{Sp}(2h+2, \mathbb{C}) \simeq \mathrm{Sp}(2h+2, \mathbb{C}) \rtimes \mathbb{Z}_2^{\mathrm{CP}} \times \mathrm{U}(1)_R$, with h being the number of either complex structure moduli or Kähler moduli. It was known that the traditional flavor symmetry was reflected by the flavor structure of Yukawa couplings, but our results suggest that the flavor symmetry G_{flavor} is enlarged to some non-Abelian groups $G_{\text{flavor}} \rtimes \mathbb{Z}_2^{\mathrm{CP}}$ by the CP symmetry on a general class of CY threefolds with standard embedding. To exemplify these results, we deal with toroidal orbifolds with and without resolutions, and three-parameter examples of CY threefolds. It turned out that three untwisted modes associated with three Kähler moduli enjoy S_4 flavor symmetry on toroidal orbifolds. On the $T^6/\mathbb{Z}_3$ and $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ orbifolds with small resolutions, there exist $(T')^3$ and S_3 symmetries among twisted modes, respectively. On the geometrical regime of $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ orbifold where the size of blow-up modes is larger than the string length, we find the S_9 flavor symmetry among blow-up models (corresponding to twisted modes in the blow-down limit). The three-parameter examples of CY threefolds

also enjoy $\mathbb{Z}_2$ and S_4 flavor symmetries as discussed in section 3.5. Hence, non-trivial flavor symmetries such as S_4 appear in not only the exact orbifold limit but also a certain class of CY threefolds. All the flavor symmetries we analyzed have an origin in the symplectic modular symmetry and are enlarged to non-Abelian groups by the CP symmetry.

In this paper, we have proposed the unification of flavor, CP, and $U(1)_R$ symmetries originated from the symplectic modular symmetry, and exemplify the flavor symmetries on CY threefolds, including toroidal results. However, there exist several future directions to pursue.

- Yukawa couplings on CY threefolds

On the toroidal backgrounds, moduli-dependent Yukawa couplings are estimated by the modular weight of matter fields, and their functional form is described by a certain modular form of $SL(2, \mathbb{Z})$ symmetry. On the other hand, the results of section 3.5 exhibit the existence of S_4 flavor symmetry of matter fields on some CY threefolds equipping the effective $SL(2, \mathbb{Z})$ modular symmetry. Hence, the Yukawa couplings including quantum corrections would be described by the modular form of S_4 flavor symmetry, controlled by the underlying symplectic modular symmetry. In this paper, we have focused on the CY moduli spaces at the classical level, but loop and instanton corrections calculated in the topological string theory appear in the prepotential as well as Yukawa couplings [73, 74]. Also, massive modes generate the higher-order couplings, which are described in an appropriate derivative of the prepotential [75]. It would be fascinating to figure out the flavor structure of matter fields, including these corrections. We hope to report on this interesting direction in the future.

- Spontaneous breaking of flavor symmetry

From the results in sections 3.3 and 3.4, there the S_3 and S_9 flavor symmetries of twisted modes on $T^6/(\mathbb{Z}_3 \times \mathbb{Z}'_3)$ orbifold with small resolutions and its geometrical regime, respectively. It indicates the spontaneous breaking of flavor symmetry would be induced by the blow-up modes. To understand the underlying structure, it is required to interpolate both the orbifold and geometrical regime. Including the stabilization of blow-up modes, we leave this topic for future research.

- Modular symmetric behavior of the twisted modes

In the limit that the size of blow-up moduli is sufficiently large, 9 twisted modes in the example of section 3.4 have S_9 flavor symmetry in $Sp(18, \mathbb{Z})$ modular symmetry. Similarly, 27 twisted modes in the example of section 3.2 may also have the S_{27} flavor symmetry in $Sp(54, \mathbb{Z})$ modular symmetry. On the other hand, the symmetry S_{27} as well as $Sp(54, \mathbb{Z})$ loses the geometrically meaning in the blow-down orbifold limit. However, twisted modes transform non-trivially under the $SL(2, \mathbb{Z})$ modular symmetry of untwisted modes because of the structure of prepotential and Kähler potential. That is a quite trivial transition of modular symmetric behavior of the twisted modes. In this paper, we have understood just two regimes, i.e., sufficiently large blow-up moduli regime ($\text{Im}(v^r) \gg 1$) and the blow-down orbifold limit ($|c^r| \ll 1$) in the context of symplectic modular symmetry. The middle regime is unclear in our analysis.

It was conjectured by ref. [76] that the blow-up moduli in both regimes would be related by $c^r \simeq \exp(2\pi i v^r)$. It is interesting to find out a similar relation of twisted matters, which brings us to understand the whole picture of modular symmetric behavior.

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A Modular form of weight 1 for T'

Following ref. [58], we define the following functions,

$$\hat{e}_1(\tau) = \frac{\eta^3(3\tau)}{\eta(\tau)}, \quad \hat{e}_2(\tau) = \frac{\eta^3(\tau/3)}{\eta(\tau)}, \quad (\text{A.1})$$

by using the Dedekind eta function $\eta(\tau)$,

$$\eta(\tau) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n), \quad (\text{A.2})$$

with $q = e^{2\pi i \tau}$. Under the T -transformation, they transform

$$\hat{e}_1 \rightarrow \omega \hat{e}_1, \quad \hat{e}_2 \rightarrow 3(1 - \omega) \hat{e}_1 + \hat{e}_2, \quad (\text{A.3})$$

with $w = e^{2\pi i/3}$. Under the S -transformation, they transform

$$\hat{e}_1 \rightarrow 3^{-3/2} i(-\tau) \hat{e}_2, \quad \hat{e}_2 \rightarrow 3^{3/2} i(-\tau) \hat{e}_1. \quad (\text{A.4})$$

By using these functions, we can construct the doublet of T' , which transforms under the T -transformation,

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} \rightarrow \rho(T) \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}, \quad (\text{A.5})$$

and under the S -transformation

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} \rightarrow (-\tau) \rho(S) \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}, \quad (\text{A.6})$$

where

$$\rho(T) = \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix}, \quad \rho(S) = -\frac{i}{\sqrt{3}} \begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & -1 \end{pmatrix}. \quad (\text{A.7})$$

We follow the representation basis in refs. [47, 48], which is different from one in ref. [58].

Explicitly, the modular form of weight 1 for the T' doublet can be written by

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} -\sqrt{2}\hat{e}_1 \\ \hat{e}_1 + \frac{1}{3}\hat{e}_2 \end{pmatrix}. \quad (\text{A.8})$$

Their q -expansions can be written by

$$\begin{aligned} x_1 &= -\sqrt{2}q^{1/3} + \dots, \\ y_1 &= 1/3 + \dots. \end{aligned} \quad (\text{A.9})$$

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