

# Grand gauge-Higgs unification on $T^2/\mathbb{Z}_3$ via the diagonal embedding method

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We study a novel six-dimensional gauge theory compactified on the  $T^2/\mathbb{Z}_3$  orbifold utilizing the diagonal embedding method. The bulk gauge group is  $G \times G \times G$ , and the diagonal part  $G^{\text{diag}}$  remains manifest in the effective four-dimensional theory. Further spontaneous breaking of the gauge symmetry occurs through the dynamics of the zero modes of the extradimensional components of the gauge field. We apply this setup to the  $SU(5)$  grand unified theory and examine the vacuum structure determined by the dynamics of the zero modes. We find bulk matter contents that radiatively induce spontaneous breakings of the unified symmetry  $G^{\text{diag}} \cong SU(5)$  down to  $SU(3) \times SU(2) \times U(1)$  at the global minima of the one-loop effective potential for the zero modes. This spontaneous breaking provides notable features such as a realization of the doublet-triplet splitting without a fine tuning and a prediction of light adjoint fields.

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## I. INTRODUCTION

Higher-dimensional gauge theory has been studied extensively as one of the attractive possibilities for physics beyond the standard model (SM). It is worth noting that the higher-dimensional gauge theory can possess the dynamical mechanism for gauge symmetry breaking via continuous Wilson line phases, called the Hosotani mechanism [1]. It is one of the promising approaches to understand the origin of the gauge symmetry breaking in the electroweak theory or in the grand unified theory (GUT) [2,3]. The former attempts are called gauge-Higgs unification [4,5]. Hence, various aspects of the higher-dimensional gauge theory with the Hosotani mechanism have been investigated.

The zero modes of the extradimensional components of the gauge field become the dynamical degrees of freedom, which behave as scalar fields at low energy [6,7]. The zero modes are closely related with the Wilson line phases, and the quantum correction generates the effective potential for the phases. The zero modes can acquire vacuum

expectation values (VEVs) at a minimum of the potential to induce the gauge symmetry breaking [1]. Interestingly, the gauge symmetry breaking patterns are definitely determined irrespective of the detail of the dynamics in the ultraviolet region thanks to the finiteness of the effective potential for the phases once we fix the content of matter fields in the theory [8,9].<sup>1</sup> One understands the definite origin of the potential that induces the gauge symmetry breaking.

The zero modes originally belong to the adjoint representation under the gauge group. Thus, it looks attractive and natural to apply the Hosotani mechanism to the spontaneous breaking of the GUT gauge symmetry such as  $SU(5)$  [2,3]. We immediately, however, encounter the difficulty that the existence of the scalar zero mode of the adjoint representation tends to be incompatible with chiral fermions, which are required in phenomenologically acceptable models. That is, if one tries to obtain the chiral fermion, the orbifold compactification with appropriate boundary conditions (BCs) is a possible framework, but the

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<sup>1</sup>Higher-loop corrections to the effective potential calculated with the bare Lagrangian generally include divergent contributions, which originate from the loop integral of sub-diagrams [9,10]. Such divergent contributions are canceled out with lower-order counterterms, and it is expected that there is no need to introduce independent counterterms to eliminate the divergent contributions [9]. In other words, in terms of the renormalized couplings, which are determined by the low-energy experiments and thus finite, instead of the bare couplings, the effective potential is free from the divergences.

scalar zero mode of the adjoint representation is projected out for the case. Thus, the  $SU(5)$  symmetry is broken by the BCs in many higher-dimensional GUT models [11]. Otherwise, an alternative direction is to consider GUT models with higher-rank gauge groups [12] that are spontaneously broken by VEVs of the scalar zero modes belonging to nonadjoint representations [13]. In these models, since the Georgi-Glashow  $SU(5)$  is broken at some fixed points on the orbifold, characteristic relations in the simple  $SU(5)$  GUT, such as the gauge coupling unification and the matter unification at a high-energy scale, are generally disturbed by  $SU(5)$  breaking localized terms on the fixed points.

The diagonal embedding method [14] makes the adjoint zero mode exist and overcomes the difficulty to apply the Hosotani mechanism to the breaking of the  $SU(5)$  symmetry accompanying the chiral fermions. Though the method is originally invented in the context of the heterotic string theory, it is possible to apply it to the higher-dimensional gauge theory. In fact, we have obtained the five-dimensional GUT models compactified on the orbifold  $S^1/\mathbb{Z}_2$ , in which the  $SU(5)$  gauge symmetry is broken down to that of the SM by the Hosotani mechanism without contradicting the existence of the chiral fermion [15]. We note that the  $SU(5)$  gauge symmetry is preserved even at the fixed points except for the effects from the Wilson line VEVs and the  $SU(5)$  breaking localized terms are absent in this case. We call the theoretical framework the type A(djoint) grand gauge-Higgs unification. Phenomenologically notable aspects in the type A grand gauge-Higgs unification with  $S^1/\mathbb{Z}_2$  compactification have been investigated [16–19]. For other types of the grand gauge-Higgs unification, referred to also as gauge-Higgs grand unification, see Ref. [5], where the Hosotani mechanism is utilized to break the electroweak symmetry.

What is striking is that the effective potential for the phases obtained in the diagonal embedding method maintains the desirable nature, that is, the finiteness. Hence, the VEV for the zero mode can be determined by minimizing the effective potential for the fixed matter content to induces the GUT gauge symmetry breaking without being affected by the physics in the ultraviolet region. Furthermore, the diagonal embedding method can straightforwardly be extended to the case with more complex orbifold compactification such as  $T^2/\mathbb{Z}_3$ .

In this paper, we shall study the gauge symmetry breaking of the six-dimensional (6D)  $SU(5)$  gauge theory compactified on the  $T^2/\mathbb{Z}_3$  in the type A grand gauge-Higgs unification. In the counterpart in the string theory for the  $\mathbb{Z}_3$  model, the gauge symmetry is realized at a level-3 affine Lie algebra or Kac-Moody algebra. We note that there is a conjecture that the generation number is a multiple of the level [20]. Though the generation number is just a free parameter set by hand within the field theory, it is meaningful to construct field theoretical models that can

be considered as effective theories of the string theoretical models with three generations. The 6D model compactified on the  $T^2/\mathbb{Z}_3$  orbifold is their simplest example. It is important and interesting to study the  $T^2/\mathbb{Z}_3$  compactification from the side of field theory. One can study the breaking of the  $SU(5)$  gauge symmetry by minimizing the one-loop effective potential for the phases. We shall determine the gauge-symmetry breaking patterns through the Hosotani mechanism for various matter contents from the one-loop effective potential and find matter contents that result the SM gauge symmetry. We also discuss phenomenological implications qualitatively such as four-dimensional (4D) chiral fermions, gauge coupling unification, fermion masses, proton decay, and so on.

This paper is organized as follows. In the next section, we introduce the basic aspects of the orbifold  $T^2/\mathbb{Z}_3$ . We discuss the field theoretical realization of the diagonal embedding method focusing on the gauge fields on the orbifold  $T^2/\mathbb{Z}_3$  in Sec. III. This section contains the fundamental ingredients for studying the gauge symmetry breaking in our model. The matter fields are introduced in Sec. IV, where the BCs and the mass spectrum are studied. We compute the effective potential for the Wilson line phases in one-loop approximation and study the gauge symmetry breaking patterns, including the breaking down to the gauge symmetry of the SM, in Secs. V and VI. We also give a brief discussion on phenomenological aspects of our model in Sec. VI. The final section is devoted to conclusions and discussions. Some details on the calculations are given in the appendixes.

## II. $T^2/\mathbb{Z}_3$ ORBIFOLD

We consider the orbifold  $T^2/\mathbb{Z}_3$  as the compact extra dimensions. To deal with coordinate vectors in  $T^2/\mathbb{Z}_3$ , it is convenient to use the basis vectors  $\mathbf{e}_i$  and the metric  $g_{ij}$ , which satisfies

$$\mathbf{e}_i \cdot \mathbf{e}_j = g_{ij}, \quad \mathbf{e}_{i+2} = -\mathbf{e}_i - \mathbf{e}_{i+1}, \quad \mathbf{e}_{i+3} = \mathbf{e}_i, \quad (2.1)$$

where  $i \in \mathbb{Z}$ . Among  $\mathbf{e}_i$ , we can choose  $\mathbf{e}_1$  and  $\mathbf{e}_2$  as a linearly independent set. A coordinate vector  $\mathbf{y}$  in  $T^2/\mathbb{Z}_3$  is spanned by the basis vector as

$$\mathbf{y} = y^i \mathbf{e}_i = y^1 \mathbf{e}_1 + y^2 \mathbf{e}_2, \quad y^i \in \mathbb{R}, \quad (2.2)$$

and it satisfies the following identifications:

$$\mathbf{y} \sim \mathbf{y} + 2\pi R \mathbf{e}_1, \quad \mathbf{y} \sim \mathbf{y} + 2\pi R \mathbf{e}_2, \quad (2.3)$$

$$\mathbf{y} = y^i \mathbf{e}_i \sim y^i \mathbf{e}_{i+1} = y^1 \mathbf{e}_2 + y^2 \mathbf{e}_3 = -y^2 \mathbf{e}_1 + (y^1 - y^2) \mathbf{e}_2, \quad (2.4)$$

where  $R$  parametrizes the size of the compact space. Contractions between upper and lower indices  $i$  imply

the summation over  $i = 1, 2$  hereafter. By requiring that the metric  $g_{ij}$  is invariant under the transformation  $e_i \rightarrow e_{i+1}$ , we can fix it as

$$\begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} = \begin{pmatrix} 1 & -1/2 \\ -1/2 & 1 \end{pmatrix}, \quad (2.5)$$

up to an overall constant, which can be absorbed into the definition of  $R$ .

The two-dimensional Cartesian coordinates, which we denote by  $x^5$  and  $x^6$ , are related to the oblique coordinates  $y^1$  and  $y^2$ . We take the basis such that  $x^5 = y^1$  and  $x^6 = 0$  hold for  $y^2 = 0$  as

$$\begin{pmatrix} x^5 \\ x^6 \end{pmatrix} = \begin{pmatrix} 1 & \cos(2\pi/3) \\ 0 & \sin(2\pi/3) \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix} = \begin{pmatrix} 1 & -1/2 \\ 0 & \sqrt{3}/2 \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix}, \quad (2.6)$$

$$\begin{aligned} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix} &= \begin{pmatrix} 1 & -\cot(2\pi/3) \\ 0 & \csc(2\pi/3) \end{pmatrix} \begin{pmatrix} x^5 \\ x^6 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 1/\sqrt{3} \\ 0 & 2/\sqrt{3} \end{pmatrix} \begin{pmatrix} x^5 \\ x^6 \end{pmatrix}, \end{aligned} \quad (2.7)$$

In light of Eqs. (2.3) and (2.4), let us introduce the operators  $\hat{T}_j$  ( $j = 1, 2$ ) and  $\hat{S}_0$  that act on the coordinates  $y^i$  as

$$\begin{aligned} \hat{T}_1 \begin{pmatrix} y^1 \\ y^2 \end{pmatrix} &= \begin{pmatrix} \hat{T}_1[y^1] \\ \hat{T}_1[y^2] \end{pmatrix} = \begin{pmatrix} y^1 + 2\pi R \\ y^2 \end{pmatrix}, \\ \hat{T}_2 \begin{pmatrix} y^1 \\ y^2 \end{pmatrix} &= \begin{pmatrix} \hat{T}_2[y^1] \\ \hat{T}_2[y^2] \end{pmatrix} = \begin{pmatrix} y^1 \\ y^2 + 2\pi R \end{pmatrix}, \end{aligned} \quad (2.8)$$

$$\hat{S}_0 \begin{pmatrix} y^1 \\ y^2 \end{pmatrix} = \begin{pmatrix} \hat{S}_0[y^1] \\ \hat{S}_0[y^2] \end{pmatrix} = \begin{pmatrix} -y^2 \\ y^1 - y^2 \end{pmatrix}. \quad (2.9)$$

The identifications in Eqs. (2.3) and (2.4) are rewritten as

$$\hat{T}_1[y^i] \sim y^i, \quad \hat{T}_2[y^i] \sim y^i, \quad \hat{S}_0[y^i] \sim y^i. \quad (2.10)$$

We can define an independent domain of the  $T^2$  torus regarding the identifications given by  $\hat{T}_1$  and  $\hat{T}_2$ , where one of the domains is shown as the gray-shaded region in Fig. 1. The additional identification given by  $\hat{S}_0$  defines the orbifold  $T^2/\mathbb{Z}_3$ , which has the fundamental domain shown in Fig. 1 by the green-shaded region.

There exist fixed points on the orbifold that are invariant up to the translations  $\hat{T}_1$  and  $\hat{T}_2$  under the discrete rotation  $\hat{S}_0$ . That is, the fixed points are given by the solution to the following equation:

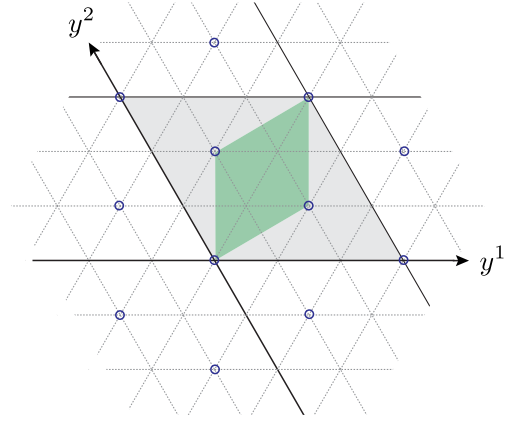


FIG. 1. The oblique coordinate system on  $T^2/\mathbb{Z}_3$ . The gray-shaded region is an independent domain of the torus  $T^2$ . The green-shaded region is a fundamental domain of the orbifold  $T^2/\mathbb{Z}_3$ . The small circles correspond to the fixed points.

$$(\hat{T}_1)^{n_1} (\hat{T}_2)^{n_2} \hat{S}_0 \begin{pmatrix} y^1 \\ y^2 \end{pmatrix} = \begin{pmatrix} y^1 \\ y^2 \end{pmatrix}, \quad \text{where } n_1, n_2 \in \mathbb{Z}. \quad (2.11)$$

We denote the three fixed points on the fundamental domain of  $T^2/\mathbb{Z}_3$  by  $y_{f(r)}^i$  ( $r = 0, 1, 2$ ), which are given by

$$\begin{aligned} \begin{pmatrix} y_{f(0)}^1 \\ y_{f(0)}^2 \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \end{pmatrix}, & \begin{pmatrix} y_{f(1)}^1 \\ y_{f(1)}^2 \end{pmatrix} &= 2\pi R \begin{pmatrix} 2/3 \\ 1/3 \end{pmatrix}, \\ \begin{pmatrix} y_{f(2)}^1 \\ y_{f(2)}^2 \end{pmatrix} &= 2\pi R \begin{pmatrix} 1/3 \\ 2/3 \end{pmatrix}. \end{aligned} \quad (2.12)$$

Any other fixed points are given by the translations of  $y_{f(r)}^i$  generated by  $\hat{T}_1$  and  $\hat{T}_2$ . In Fig. 1, the fixed points are shown by the small circles.

The operators  $\hat{T}_1$ ,  $\hat{T}_2$ , and  $\hat{S}_0$  satisfy

$$\hat{T}_1 \hat{T}_2 = \hat{T}_2 \hat{T}_1, \quad \hat{S}_0 \hat{T}_1 = \hat{T}_2 \hat{S}_0. \quad (2.13)$$

Thus,  $\hat{T}_1$ ,  $\hat{T}_2$ , and  $\hat{S}_0$  are not independent to each other. In addition, it is convenient to define

$$\hat{S}_1 \equiv \hat{T}_1 \hat{S}_0, \quad \hat{S}_2 \equiv \hat{T}_2 \hat{T}_1 \hat{S}_0, \quad (2.14)$$

where  $\hat{S}_r^3 = \hat{I}$  for  $r = 0, 1, 2$  and  $\hat{I}[y^i] = y^i$ . The operators  $\hat{S}_r$  give  $2\pi/3$  rotations around the fixed points  $y_{f(r)}^i$  and satisfy  $\hat{S}_r[y_{f(r)}^i] = y_{f(r)}^i$ . Among the above operators, we can choose  $\hat{T}_1$  and  $\hat{S}_0$  as the independent ones, and the others  $\hat{T}_2$ ,  $\hat{S}_1$ , and  $\hat{S}_2$  can be expressed by  $\hat{T}_1$  and  $\hat{S}_0$ .

It is useful to introduce the dual basis vectors  $\tilde{e}^i$  as

$$\tilde{e}^i \cdot e_j = \delta_j^i, \quad \tilde{e}^i \cdot \tilde{e}^j = g^{ij}, \quad g^{ik}g_{kj} = \delta_j^i, \quad (2.15)$$

where  $\delta_j^i$  is the Kronecker delta and

$$\begin{pmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{pmatrix} = \frac{4}{3} \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}. \quad (2.16)$$

Note that  $g^{ij}e_j = \tilde{e}^i$  and  $g_{ij}\tilde{e}^j = e_i$  hold. We can introduce a dual vector  $\tilde{\mathbf{k}}$  that is spanned by the dual basis vectors as

$$\tilde{\mathbf{k}} = k_1\tilde{e}^1 + k_2\tilde{e}^2, \quad k_i \in \mathbb{R}. \quad (2.17)$$

Then, one sees  $\tilde{\mathbf{k}} \cdot \mathbf{y} = k_i y^i \in \mathbb{R}$ . As discussed in Appendix A,  $\tilde{e}^i$  is a natural basis for a Kalzua-Klein (KK) discretized momentum, which is mapped to a point on the lattice spanned by  $\tilde{e}^i$  in a normalization.

The identification in Eq. (2.4) is related to the basis change  $e_i \rightarrow e_{i+1}$ . Under the basis change, the dual basis vectors also change  $\tilde{e}^i \rightarrow \tilde{e}^i$ . Requiring  $e_{i+1} \cdot \tilde{e}^i = \delta_j^i$ , we obtain  $\tilde{e}^1 = -\tilde{e}^1 + \tilde{e}^2$  and  $\tilde{e}^2 = -\tilde{e}^1$ . Thus, corresponding to Eq. (2.4), we obtain the identification for the dual vector as

$$\tilde{\mathbf{k}} = k_i \tilde{e}^i \sim k_1(-\tilde{e}^1 + \tilde{e}^2) + k_2(-\tilde{e}^1) = (-k_1 - k_2)\tilde{e}^1 + k_1\tilde{e}^2. \quad (2.18)$$

Then, the action of the operator  $\hat{S}_0$  on the coordinates of dual vectors is naturally defined by

$$\hat{S}_0[k_i] = k_{i-1}, \quad (2.19)$$

where we have also defined

$$k_0 = -k_1 - k_2, \quad k_{i+3} = k_i, \quad i \in \mathbb{Z}. \quad (2.20)$$

From the above, one sees  $\hat{S}_0[k_i]\hat{S}_0[y^i] = k_i y^i$  and

$$k_i \hat{S}_0[y^i] = \hat{S}_0^{-1}[k_i] y^i = k_{i+1} y^i. \quad (2.21)$$

We use Eq. (2.21) for deriving the KK expansions of fields discussed in Appendix A.

### III. THE DIAGONAL EMBEDDING METHOD ON $M^4 \times T^2/\mathbb{Z}_3$ : GAUGE FIELDS

#### A. Lagrangian for gauge fields

We start to discuss the gauge theory with the field-theoretical realization of the diagonal embedding method on  $M^4 \times T^2/\mathbb{Z}_3$ , where  $M^4$  is the Minkowski spacetime. In the following, we denote the 6D orthogonal coordinates by  $x^M = (x^\mu, x^5, x^6)$  ( $\mu = 0, 1, 2, 3$ ). For the extradimensional

coordinates, we also use the oblique coordinates  $y^1$  and  $y^2$  in Eq. (2.7) instead of  $x^5$  and  $x^6$ . The metric of  $M^4 \times T^2/\mathbb{Z}_3$  is defined such that  $x^M x_M = \eta_{\mu\nu}^4 x^\mu x^\nu - g_{ij} y^i y^j$ , where  $\eta_{\mu\nu}^4 = \text{diag}(1, -1, -1, -1)$  and  $g_{ij}$  is given in Eq. (2.5).

The action is given by the Lagrangians for the gauge fields  $\mathcal{L}_{\text{YM}}$  and the matter fields  $\mathcal{L}_{\text{mat}}$ , which will be discussed in the next section, as

$$S = \int_0^{2\pi R} dy^1 \int_0^{2\pi R} dy^2 \sqrt{\det g_{ij}} \int d^4 x \mathcal{L}, \quad \mathcal{L} = \mathcal{L}_{\text{YM}} + \mathcal{L}_{\text{mat}}, \quad (3.1)$$

where  $\det g_{ij} = 3/4$ . The diagonal embedding method on the orbifold requires that the theory respects three copies of gauge symmetry  $G$  and the global symmetry  $\mathbb{Z}_3^{(\text{ex})}$  that permutes the three copies cyclically. Therefore, let us introduce the Lagrangian for the gauge fields as

$$\begin{aligned} \mathcal{L}_{\text{YM}} &= -\frac{1}{2} \sum_{k=1}^3 \text{Tr}(F_{MN}^{(k)} F^{(k)MN}), \\ F_{MN}^{(k)} &= \partial_M A_N^{(k)} - \partial_N A_M^{(k)} + ig[A_M^{(k)}, A_N^{(k)}], \end{aligned} \quad (3.2)$$

where  $g$  is the gauge coupling constant. The gauge fields  $A_M^{(k)}$  ( $k = 1, 2, 3$ ) are expanded by the generators of the gauge symmetry as  $A_M^{(k)} = A_M^{(k)a} t_a^{(k)}$ , where the indices  $a$  run from 1 to the dimension of the Lie algebra of  $G$ , and the summation over  $a$  is implied. The operators  $t_a^{(k)}$  ( $k = 1, 2, 3$ ) are representation matrices of the generators. We adopt the convention that the matrices satisfy the following relations:

$$[t_a^{(k)}, t_b^{(k')}] = if_{ab}^c t_c^{(k)} \delta^{kk'}, \quad \text{Tr}[t_a^{(k)} t_b^{(k')}] = \frac{1}{2} \delta_{ab} \delta^{kk'}, \quad (3.3)$$

where  $f_{ab}^c$  is the structure constant. In Eqs. (3.2) and (3.3), the trace is taken over the representation space.

The Lagrangian in Eq. (3.2) has the gauge symmetry  $G \times G \times G$  and the global symmetry  $\mathbb{Z}_3^{(\text{ex})}$ . We define the gauge transformation of the gauge field as

$$A_M^{(k)} \rightarrow \Omega^{(k)} \left( A_M^{(k)} - \frac{i}{g} \partial_M \right) \Omega^{(k)\dagger}, \quad \Omega^{(k)} = \exp(ig\alpha^{(k)a} t_a^{(k)}), \quad (3.4)$$

where  $\alpha^{(k)a}(x)$  are gauge parameters. To define the global  $\mathbb{Z}_3^{(\text{ex})}$  transformation of the gauge field, it is helpful to extend the range of index  $k \in \{1, 2, 3\}$  to  $k \in \mathbb{Z}$  and to introduce the periodicity for the index  $k$ , e.g.,  $A_N^{(k+3)a} = A_N^{(k)a}$  and  $t_a^{(k+3)} = t_a^{(k)}$ . Hereafter, we use this notation. Then, we can write the global  $\mathbb{Z}_3^{(\text{ex})}$  transformation of the gauge field as follows:

$$A_M^{(k)} = A_M^{(k)a} t_a^{(k)} \xrightarrow{\mathbb{Z}_3^{(\text{ex})}} A_M^{(k+1)a} t_a^{(k)}. \quad (3.5)$$

Under the transformations in Eqs. (3.4) and (3.5), the Lagrangian in Eq. (3.2) is invariant.

Using the above notation, we can define  $A_M^{[p]a}$  that are the eigenstates of the transformation in Eq. (3.5) as

$$A_M^{[p]a} = \frac{1}{\sqrt{3}} \sum_{k=1}^3 \omega^{-kp} A_M^{(k)a}, \quad A_M^{(k)a} = \frac{1}{\sqrt{3}} \sum_{p=-1}^1 \omega^{kp} A_M^{[p]a}, \quad (3.6)$$

where  $p \in \mathbb{Z}$  and  $\omega = e^{2\pi i/3}$ . From the above definition,  $A_M^{[p+3]a} = A_M^{[p]a}$  and  $(A_M^{[p]a})^* = A_M^{[-p]a}$  hold. Note that  $A_M^{[p]a}$  has the eigenvalue of  $\omega^p$  under the  $\mathbb{Z}_3^{(\text{ex})}$  transformation in Eq. (3.5).

### B. Orbifold boundary conditions and residual gauge symmetries

In theories on the orbifold, field values are constrained since the extradimensional coordinates obey the identifications discussed in the previous section. To clarify the constraints, we define the BCs [21] for the gauge fields. As discussed in Sec. II, we treat  $\hat{T}_1$  and  $\hat{S}_0$  as the independent operators and define the BCs for the gauge fields  $A_M^{(k)a}(x^\mu, y^i)$  as follows:

$$\begin{aligned} A_\mu^{(k)a}(x^\mu, \hat{T}_1[y^i]) &= A_\mu^{(k)a}(x^\mu, y^i), \\ A_\mu^{(k)a}(x^\mu, \hat{S}_0[y^i]) &= A_\mu^{(k+1)a}(x^\mu, y^i), \end{aligned} \quad (3.7)$$

$$\begin{aligned} A_{y^i}^{(k)a}(x^\mu, \hat{T}_1[y^i]) &= A_{y^i}^{(k)a}(x^\mu, y^i), \\ A_{y^i}^{(k)a}(x^\mu, \hat{S}_0[y^i]) &= A_{y^{i-1}}^{(k+1)a}(x^\mu, y^i), \end{aligned} \quad (3.8)$$

where  $A_{y^1}^{(k)a} = A_5^{(k)a}$ ,  $A_{y^2}^{(k)a} = -\frac{1}{2}A_5^{(k)a} + \frac{\sqrt{3}}{2}A_6^{(k)a}$ , and  $A_{y^0}^{(k)a} = -A_{y^1}^{(k)a} - A_{y^2}^{(k)a}$ . Hereafter, we also use the notation  $A_{y^{i+3}}^{(k)a} = A_{y^i}^{(k)a}$  ( $i \in \mathbb{Z}$ ).

In general, BCs can nontrivially act on the representation space of not only the discrete group  $\mathbb{Z}_3^{(\text{ex})}$  but also the gauge group  $G$ . Nevertheless, it should be emphasized that we can always take the trivial BCs for  $G$  as in Eqs. (3.7) and (3.8) without loss of generality. This is understood as follows. Although one can introduce nontrivial transformations in the representation space of  $G$  [21,22], which we here call the gauge twists, the nontrivial gauge twists do not affect the low-energy physics in the present case. For the gauge twist with respect to  $\hat{S}_0$ , this introduces just a difference among the bases in the representation space of the generators  $t_a^{(1)}$ ,  $t_a^{(2)}$ , and  $t_a^{(3)}$ . Such difference can always be absorbed into the redefinition of the generators  $t_a^{(k)}$ . The

gauge twist with respect to  $\hat{T}_1$  can be absorbed by the continuous Wilson line phases [22], which will be discussed in detail in the next section, through the gauge transformations with the gauge parameters depending on the extradimensional coordinates. Then, if the BCs are the same up to the gauge twist with respect to  $\hat{T}_1$ , these BCs are said to belong to the same equivalence class [23–25]. As seen below, the vacuum is determined by a nontrivial expectation value of the Wilson line phases. It is known that BCs in an equivalence class describe the same low-energy physics through the dynamics of the Wilson line phases determined by the effective potential generated by quantum corrections [24].<sup>2</sup>

From the BCs and Eq. (3.6), it follows that

$$\begin{aligned} A_\mu^{[p]a}(x^\mu, \hat{T}_1[y^i]) &= A_\mu^{[p]a}(x^\mu, y^i), \\ A_\mu^{[p]a}(x^\mu, \hat{S}_0[y^i]) &= \omega^p A_\mu^{[p]a}(x^\mu, y^i), \end{aligned} \quad (3.9)$$

$$\begin{aligned} A_{y^i}^{[p]a}(x^\mu, \hat{T}_1[y^i]) &= A_{y^i}^{[p]a}(x^\mu, y^i), \\ A_{y^i}^{[p]a}(x^\mu, \hat{S}_0[y^i]) &= \omega^p A_{y^{i-1}}^{[p]a}(x^\mu, y^i). \end{aligned} \quad (3.10)$$

The  $\mathbb{Z}_3$  transformation of  $y^i$  generated by  $\hat{S}_0$  is discussed in Sec. II and is contained in  $SO(2)$  rotations that are part of the 6D Lorentz transformation. Hence, the extradimensional components of the gauge field nontrivially transform under the  $\mathbb{Z}_3$  transformation, and thus  $A_{y^i}^{[p]a}$  are not the eigenstates of the BC for  $\hat{S}_0$  in Eq. (3.10). We refer to the  $\mathbb{Z}_3$  subgroup of the  $SO(2)$  as  $\mathbb{Z}_3^{(L)}$ . Let us denote the eigenstates of the  $\mathbb{Z}_3^{(L)}$  transformation by  $A_{[q]}^{(k)a}$  that are defined as

$$A_{[q]}^{(k)a} = \frac{1}{3} \sum_{\ell=1}^3 \omega^{-(\ell-1)q} A_{y^\ell}^{(k)a}, \quad A_{y^\ell}^{(k)a} = \sum_{q=1}^3 \omega^{(\ell-1)q} A_{[q]}^{(k)a}, \quad (3.11)$$

where  $q \in \mathbb{Z}$  and the superscript of  $y^\ell$  takes  $\ell = 1, 2, 3$ , whereas that of  $y^i$  takes  $i = 1, 2$  as explained in Sec. II. The normalization in Eq. (3.11) is fixed by  $A_{[\pm 1]}^{(k)a} = (A_5^{(k)a} \mp iA_6^{(k)a})/2$ , which correspond to the gauge fields  $A_z^{(k)a}$  and  $A_{\bar{z}}^{(k)a}$  associated with the complex coordinates  $z = x^5 + ix^6$  and  $\bar{z} = x^5 - ix^6$ . With this definition, we find  $A_{[q+3]}^{(k)a} = A_{[q]}^{(k)a}$ ,  $(A_{[q]}^{(k)a})^* = A_{[-q]}^{(k)a}$ , and  $A_{[0]}^{(k)a} = 0$ . For fixed  $k$  and  $a$ , there are two real degrees of freedom in  $A_{[q]}^{(k)a}$  as in  $A_{y^i}^{(k)a}$ . From Eq. (3.8), the BC for  $A_{[q]}^{(k)a}$  is given by

<sup>2</sup>We introduce the twist for  $\mathbb{Z}_3^{(\text{ex})}$  only associated with  $\hat{S}_0$  in Eqs. (3.7) and (3.8). One may consider a  $\mathbb{Z}_3^{(\text{ex})}$  twist associated with  $\hat{T}_1$ , which cannot be absorbed by the Wilson line phases.

$$A_{[q]}^{(k)a}(x^\mu, \hat{S}_0[y^i]) = \omega^{-q} A_{[q]}^{(k+1)a}(x^\mu, y^i). \quad (3.12)$$

Namely  $A_{[q]}^{(k)a}$  has the eigenvalue  $\omega^{-q}$  under the  $\mathbb{Z}_3^{(L)}$  transformation.

From the above discussions, the eigenstates  $A_{[q]}^{[p]a}$  of the BCs are naturally defined as

$$A_{[q]}^{[p]a} = \frac{1}{\sqrt{3}} \sum_{k=1}^3 \omega^{-kp} A_{[q]}^{(k)a} = \frac{1}{3\sqrt{3}} \sum_{\ell=1}^3 \sum_{k=1}^3 \omega^{-kp-(\ell-1)q} A_{y^\ell}^{(k)a}. \quad (3.13)$$

Inversely, it also follows that

$$A_{y^\ell}^{(k)a} = \frac{1}{\sqrt{3}} \sum_{p=-1}^1 \sum_{q=-1}^1 \omega^{(\ell-1)q+kp} A_{[q]}^{[p]a}. \quad (3.14)$$

Then,  $A_{[\pm 1]}^{[p]a}$  satisfies the BCs as

$$\begin{aligned} A_{[\pm 1]}^{[p]a}(x^\mu, \hat{T}_1[y^i]) &= A_{[\pm 1]}^{[p]a}(x^\mu, y^i), \\ A_{[\pm 1]}^{[p]a}(x^\mu, \hat{S}_0[y^i]) &= \omega^{p \mp 1} A_{[\pm 1]}^{[p]a}(x^\mu, y^i). \end{aligned} \quad (3.15)$$

From the BCs in Eqs. (3.9) and (3.15), it is implied that  $A_\mu^{[0]a}$ ,  $A_{[1]}^{[1]a}$ , and  $A_{[-1]}^{[-1]a}$  have zero modes, which do not have  $\mathcal{O}(1/R)$  KK masses in the 4D effective theory.

We remind that the Lagrangian possesses  $\mathbb{Z}_3^{(\text{ex})}$  and  $\mathbb{Z}_3^{(L)}$  symmetries. The gauge field  $A_{[q]}^{[p]a}$  has the charges  $\omega^p$  and  $\omega^{-q}$  under the  $\mathbb{Z}_3^{(\text{ex})}$  and  $\mathbb{Z}_3^{(L)}$  transformations, respectively. We can rearrange the two  $\mathbb{Z}_3$  symmetries as  $\mathbb{Z}_3^{(+)}$  and  $\mathbb{Z}_3^{(-)}$ , under which transformations  $A_{[q]}^{[p]a}$  has the charges  $\omega^{p-q}$  and  $\omega^{p+q}$ , respectively. The BCs for  $\hat{S}_0$  introduced in Eqs. (3.7) and (3.8) are regarded as the twist for  $\mathbb{Z}_3^{(+)}$ , and the zero mode is neutral under  $\mathbb{Z}_3^{(+)}$ .

The BCs determine the zero modes of the gauge field. The low-energy gauge symmetry associated with the zero modes of the 4D component of the gauge field is referred to as the residual gauge symmetry. To clarify the residual gauge symmetry, we focus on the covariant derivative,

$$D_\mu = \partial_\mu + ig \sum_{k=1}^3 A_\mu^{(k)a} t_a^{(k)} = \partial_\mu + i\tilde{g} \sum_{p=-1}^1 A_\mu^{[p]a} t_a^{[p]}, \quad (3.16)$$

where we have introduced

$$t_\mu^{[p]} = \sum_{k=1}^3 \omega^{-kp} t_a^{(k)}, \quad t_a^{(k)} = \frac{1}{3} \sum_{p=-1}^1 \omega^{kp} t_a^{[p]}, \quad \tilde{g} = \frac{g}{\sqrt{3}}. \quad (3.17)$$

The generator  $t_a^{[p]}$  has a proper normalization and satisfies

$$[t_a^{[p]}, t_b^{[p']}] = if_{ab}{}^c t_c^{[p+p']}. \quad (3.18)$$

As mentioned above,  $A_\mu^{[0]a}$  have zero modes. At a low-energy regime,  $A_\mu^{[1]a}$  and  $A_\mu^{[-1]a}$  are decoupled from the effective theory since they have no zero modes. Hence, the residual gauge symmetry is the diagonal part of  $G \times G \times G$  generated by  $t_a^{[0]} = t_a^{(1)} + t_a^{(2)} + t_a^{(3)}$ . We denote this diagonal part by  $G^{\text{diag}}$ . From the commutation relation in Eq. (3.18) for  $p=0$  and  $p'=\pm 1$ , we see that  $t_a^{[\pm 1]}$  transforms as the adjoint representation under the residual gauge symmetry  $G^{\text{diag}}$ .

### C. Wilson line phases and spontaneous symmetry breaking

Let us focus on the zero mode of the extradimensional component of the gauge field. As discussed in the previous subsection,  $A_{[1]}^{[1]a}$  and  $A_{[-1]}^{[-1]a}$  have zero modes. They carry continuous Wilson line degrees of freedom and can develop nonzero VEVs to break the gauge symmetry spontaneously. We introduce the parametrization as

$$\langle A_{[1]}^{[1]a} \rangle \equiv \frac{1}{R\tilde{g}} a_z^a, \quad \langle A_{[-1]}^{[-1]a} \rangle = \langle A_{[1]}^{[1]a} \rangle^* = \frac{1}{R\tilde{g}} a_z^{a*}, \quad (3.19)$$

where  $a_z^a$  is a complex parameter. Except for the above,  $\langle A_{[\pm 1]}^{[p]a} \rangle = 0$  is satisfied. We also introduce the parametrization of the VEVs of  $A_{y^\ell}^{(k)a}$  as

$$\langle A_{y^\ell}^{(k)a} \rangle = \frac{1}{Rg} (\omega^{k+\ell-1} a_z^a + \bar{\omega}^{k+\ell-1} a_z^{a*}) \equiv \frac{2}{Rg} \tilde{a}_{k+\ell}^a, \quad (3.20)$$

here  $\bar{\omega} = e^{-2\pi i/3}$ . The real part of  $\omega^{k+\ell-1} a_z^a$  is equal to  $\tilde{a}_{k+\ell}^a$ .<sup>3</sup> From Eq. (3.20), one sees that  $\tilde{a}_{k+\ell}^a$  has the periodicity under the shift of its subscript as  $\tilde{a}_{k+\ell+3}^a = \tilde{a}_{k+\ell}^a$ .

Let us consider the Wilson line phases defined with closed paths on the orbifold  $T^2/\mathbb{Z}_3$ . We denote the three distinct noncontractible cycles by  $C_\ell$  ( $\ell=1, 2, 3$ ). The cycle  $C_1$  is defined by the path from  $y^1=0$  to  $2\pi R$ , while keeping  $y^2=0$ . The cycle  $C_2$  is defined by the path from  $y^2=0$  to  $2\pi R$ , while keeping  $y^1=0$ . The cycle  $C_3$  is defined by the path from  $-y^1-y^2=0$  to  $2\pi R$ , while keeping  $y^1=y^2$ . By using them, we define the Wilson line phase factors  $W_\ell$  as

<sup>3</sup>We have determined the normalization of  $\tilde{a}_{k+\ell}^a$  in Eq. (3.20) so that the Wilson line phase factors defined in Eq. (3.21) are invariant under integer shifts of  $\tilde{a}_{k+\ell}^a$  in the  $G = SU(N)$  case where the length of the root vectors are taken to be 1. Namely, the Cartan generator  $H$  in the fundamental representation of the  $SU(2)$  Lie algebra associated with a root vector is chosen as  $H = \text{diag}(1, -1)/2$ .

$$\begin{aligned}
W_\ell &\equiv \exp\left(ig \sum_{k=1}^3 \oint_{C_\ell} dy^i \langle A_{y^i}^{(k)a} \rangle t_a^{(k)}\right) \\
&= \exp\left(2\pi ig R \sum_{k=1}^3 \langle A_{y^\ell}^{(k)a} \rangle t_a^{(k)}\right) \quad (3.21)
\end{aligned}$$

$$\equiv \exp[i(\Theta_\ell + \Theta_\ell^\dagger)], \quad (3.22)$$

where  $\ell = 1, 2, 3$ , and we also define the Wilson line phases  $\Theta_\ell$  as

$$\Theta_\ell = 2\pi\omega^{\ell-1} a_z^a t_a^{[-1]}. \quad (3.23)$$

From the above, we find  $\Theta_{\ell+k} = \omega^k \Theta_\ell$ , which implies  $\Theta_1 + \Theta_2 + \Theta_3 \propto 1 + \omega + \bar{\omega} = 0$ . Let us note that the phase factors in Eq. (3.21) have physical consequences, rather than the phases in Eq. (3.23) [26].

The Wilson line phases are invariant under  $\mathbb{Z}_3^{(+)}$  since the phases depend on the VEVs of  $A_{[p]}^{[p]a}$  ( $p = \pm 1$ ), which is neutral under  $\mathbb{Z}_3^{(+)}$ . On the other hand,  $A_{[p]}^{[p]a}$  has the eigenvalue  $\omega^{2p}$  under  $\mathbb{Z}_3^{(-)}$ . One sees that the gauge fields and the phases transform as  $\langle A_{y^\ell}^{(k)a} \rangle \rightarrow \langle A_{y^{\ell+1}}^{(k+1)a} \rangle$  and  $\tilde{a}_{k+\ell}^a \rightarrow \tilde{a}_{k+\ell-1}^a$  under  $\mathbb{Z}_3^{(-)}$ . This implies the transformation law of the phase factors,  $W_\ell \rightarrow W_{\ell-1}$ , under  $\mathbb{Z}_3^{(-)}$ . Thus, the symmetry  $\mathbb{Z}_3^{(-)}$  is generally broken by nontrivial VEVs of the Wilson line phases. Notice that, if  $W_1 = W_2 = W_3$  is satisfied, the symmetry  $\mathbb{Z}_3^{(-)}$  survives. Thus, the vacuum with the alignment  $W_1 = W_2 = W_3$  is discriminated in view of the symmetry and is provided by  $\tilde{a}_\ell^a - \tilde{a}_{\ell+1}^a = 0 \pmod{1}$ .

The VEVs of the Wilson line phases are dynamically determined. Thus, we focus on the potential for the zero mode of  $A_{y^i}^{(k)a}$ . In the present case,  $\mathcal{L}_{\text{YM}}$  involves the nonvanishing potential for  $A_{y^i}^{(k)a}$  at the classical level.<sup>4</sup> From Eqs. (3.2) and (3.3), we obtain

$$\begin{aligned}
\mathcal{L}_{\text{YM}} &\ni -\frac{1}{2} g^{i\ell} g^{jj'} \text{Tr} \left( \sum_{k=1}^3 F_{y^i y^j}^{(k)} \sum_{k'=1}^3 F_{y^{i'} y^{j'}}^{(k')} \right) \\
&= -\frac{4}{3} \text{Tr} \left( \sum_{k=1}^3 F_{y^1 y^2}^{(k)} \sum_{k'=1}^3 F_{y^1 y^2}^{(k')} \right). \quad (3.24)
\end{aligned}$$

The VEVs of the field strength tensors are written by the Wilson line phases as

<sup>4</sup>In five-dimensional models compactified on the  $S^1/\mathbb{Z}_2$  orbifold, there is no tree-level potential only for the zero modes of the extradimensional components of the gauge field, although the zero modes can have tree-level potentials in supersymmetric models with the helps of additional scalars belonging to vector multiplets [27].

$$\begin{aligned}
\sum_{k=1}^3 \langle F_{y^i y^j}^{(k)} \rangle &= ig \left[ \sum_{k=1}^3 \langle A_{y^i}^{(k)a} \rangle t_a^{(k)}, \sum_{k'=1}^3 \langle A_{y^j}^{(k')a} \rangle t_a^{(k')} \right] \\
&= \frac{i}{(2\pi R)^2 g} [\Theta_i + \Theta_i^\dagger, \Theta_j + \Theta_j^\dagger], \quad (3.25)
\end{aligned}$$

where we have used Eq. (3.23). Therefore, the tree-level potential for the Wilson line phases is given by

$$\begin{aligned}
V_{\text{tree}} &\equiv \frac{4}{3(2\pi R)^4 g^2} \text{Tr}(\mathcal{F}_\Theta \mathcal{F}_\Theta^\dagger), \quad \text{where} \\
\mathcal{F}_\Theta &= [\Theta_1 + \Theta_1^\dagger, \Theta_2 + \Theta_2^\dagger] = (\bar{\omega} - \omega)[\Theta_1, \Theta_1^\dagger]. \quad (3.26)
\end{aligned}$$

Note that the tree-level potential is positive definite and has flat directions. On the flat directions,  $[\Theta_1, \Theta_1^\dagger] = 0$  is satisfied, and hence the potential is minimized as  $V_{\text{tree}} = 0$ . In this case,  $W_1 W_2 W_3 = e^{i\Theta_1 + \Theta_2 + \Theta_3} e^{i\Theta_1^\dagger + \Theta_2^\dagger + \Theta_3^\dagger} = 1$  is satisfied.

There are quantum corrections to the effective potential for the phases. As discussed above, the tree-level potential is minimized along the flat directions. Due to the loop factors, the quantum corrections are generally suppressed compared to the tree-level contribution if it is nonvanishing. For the quadratic terms, it is vanishing even along the nonflat direction.<sup>5</sup> Thus, we approximate that the minimum resides in the flat direction and  $[\Theta_1, \Theta_1^\dagger] = 0$  holds even if the quantum corrections are incorporated. In this case, we can diagonalize  $\Theta_\ell$  by  $G^{\text{diag}}$  transformations without loss of generality.

The flat direction of the tree-level potential is no longer flat in the effective potential. If some nontrivial values of the phase degrees of freedom  $\Theta_\ell + \Theta_\ell^\dagger$  are determined by the quantum corrections to the potential, the residual symmetry  $G^{\text{diag}}$  is spontaneously broken to  $G_0$ , whose elements and the Lie algebra  $\mathfrak{g}_0$  are given by

$$\begin{aligned}
G_0 &= \{ e^{i\alpha^a t_a^{[0]}} | t_a^{[0]} \in \mathfrak{g}_0, \alpha^a \in \mathbb{R} \}, \quad \text{where} \\
\mathfrak{g}_0 &= \{ t_a^{[0]} | [t_a^{[0]}, W_j] = 0 \text{ for } j = 1, 2 \}. \quad (3.27)
\end{aligned}$$

In this case, the zero modes of the gauge fields  $A_\mu^{[0]a}$ , which is related to the broken generators corresponding to  $G^{\text{diag}}/G_0$ , acquire masses at low energy. This is understood as follows. By using  $y^i$ -dependent gauge transformations, we can always choose a gauge such that nontrivial VEVs of  $A_{[p]}^{[p]a}$  are gauged away. After the gauge transformations, the BC for  $A_\mu^{[0]a}$  related to the translation by  $\hat{T}_j$  is changed

<sup>5</sup>These quadratic terms are contained in tadpole terms of the field strength, which are generally generated on the fixed points [28]. In the present model, as long as  $G$  of the bulk gauge group  $G \times G \times G$  is semisimple, such tadpole terms are forbidden because  $G$  remains unbroken on the fixed points.

to  $A_\mu^{[0]a}(x^\mu, \hat{T}_j[y^i])t_a^{[0]} = W_j A_\mu^{[0]a}(x^\mu, y^i)t_a^{[0]} W_j^\dagger$  ( $j = 1, 2$ ). Thus, the zero modes of  $A_\mu^{[0]a}$  of the broken generators are projected out. In this way, the spontaneous symmetry breaking can generally be triggered by nontrivial VEVs of Wilson line phases.

Since  $\Theta_\ell + \Theta_\ell^\dagger$  is diagonal, we can expand them by the elements of Cartan subalgebra  $\mathfrak{h} \in \mathfrak{g}$ , where  $\mathfrak{g}$  is the Lie algebra of  $G$ . We denote the generators in  $\mathfrak{h}$  by  $H_{\hat{a}}$  ( $\hat{a} = 1, \dots, r$ ), where  $r$  is the rank of  $\mathfrak{g}$ . Hence, we obtain

$$\Theta_\ell + \Theta_\ell^\dagger = 2\pi Rg \sum_{k=1}^3 \langle A_{y^\ell}^{(k)\hat{a}} \rangle H_{\hat{a}}^{(k)} = 2\pi \sum_{k=1}^3 \tilde{a}_{k+\ell}^{\hat{a}} 2H_{\hat{a}}^{(k)}, \quad (3.28)$$

$$W_\ell = \exp(2\pi i \tilde{a}_{\ell+1}^{\hat{a}} 2H_{\hat{a}}^{(1)}) \otimes \exp(2\pi i \tilde{a}_{\ell+2}^{\hat{a}} 2H_{\hat{a}}^{(2)}) \otimes \exp(2\pi i \tilde{a}_\ell^{\hat{a}} 2H_{\hat{a}}^{(3)}). \quad (3.29)$$

To determine the VEVs of the Wilson line phases, we should evaluate the effective potential for  $\tilde{a}_\ell^{\hat{a}}$ . The quantum corrections to the effective potential depend on the matter contents of the theory. Thus, we discuss bulk matter fields in the next section, and the one-loop corrections are studied in Sec. V.

#### IV. THE DIAGONAL EMBEDDING METHOD ON $M^4 \times T^2/\mathbb{Z}_3$ : BULK MATTER FIELDS

Let us start to discuss bulk matter fields. The invariance of the Lagrangian under the  $\mathbb{Z}_3^{(\text{ex})}$  transformation restricts the matter contents of the theory. We denote the representation of a matter field under the bulk gauge symmetry  $G \times G \times G$  by  $(\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3)$ . In order to preserve the  $\mathbb{Z}_3^{(\text{ex})}$  symmetry of the theory, matter fields should be incorporated as the set of the representations  $(\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3)$ ,  $(\mathcal{R}_3, \mathcal{R}_1, \mathcal{R}_2)$ , and  $(\mathcal{R}_2, \mathcal{R}_3, \mathcal{R}_1)$ . We refer to this set of fields as a  $\mathbb{Z}_3^{(\text{ex})}$  *threefold*. However, there is an exception; if a field belongs to the representation of  $\mathcal{R}_1 = \mathcal{R}_2 = \mathcal{R}_3$ , we can incorporate a single field keeping  $\mathbb{Z}_3^{(\text{ex})}$ . We refer to the field of the type  $(\mathcal{R}, \mathcal{R}, \mathcal{R})$  as a  $\mathbb{Z}_3^{(\text{ex})}$  *onefold*.

##### A. Lagrangian for bulk scalar fields

As the simplest example, we first discuss a threefold scalar  $\Phi_{\mathcal{R}}^{(k)}$  ( $k = 1, 2, 3$ ), which belongs to the following representation:

$$\Phi_{\mathcal{R}}^{(1)} \sim (\mathcal{R}, \mathbf{1}, \mathbf{1}), \quad \Phi_{\mathcal{R}}^{(2)} \sim (\mathbf{1}, \mathcal{R}, \mathbf{1}), \quad \Phi_{\mathcal{R}}^{(3)} \sim (\mathbf{1}, \mathbf{1}, \mathcal{R}), \quad (4.1)$$

where  $\mathbf{1}$  means the singlet under  $G$ . Their components are denoted by  $(\Phi_{\mathcal{R}}^{(k)})_\alpha$ , where  $\alpha$  runs 1 to  $\dim(\mathcal{R})$ . Under the

$\mathbb{Z}_3^{(\text{ex})}$  transformation, the threefold scalar can be defined to transform as  $(\Phi_{\mathcal{R}}^{(k)})_\alpha \rightarrow \omega^p (\Phi_{\mathcal{R}}^{(k+1)})_\alpha$ , where  $p \in \{0, \pm 1\}$ . Here, we introduce the notation  $\Phi_{\mathcal{R}}^{(k+3)} \equiv \Phi_{\mathcal{R}}^{(k)}$  ( $k \in \mathbb{Z}$ ) for convenience. For a real field such as the gauge field, the integer  $p$  should be 0. For the complex scalars, the phase factor  $\omega^p$  can be absorbed by redefinitions of  $(\Phi_{\mathcal{R}}^{(k)})_\alpha$ . From the above definitions, one sees that the following Lagrangian is  $\mathbb{Z}_3^{(\text{ex})}$  invariant:

$$\mathcal{L}(\Phi_{\mathcal{R}}^{(k)}) \equiv \sum_{k=1}^3 |(D_M^{(k)})_\alpha^\beta (\Phi_{\mathcal{R}}^{(k)})_\beta|^2, \quad (D_M^{(k)})_\alpha^\beta = \partial_M \delta_\alpha^\beta + ig A_M^{(k)a} (T_a^{[\mathcal{R}]})_\alpha^\beta, \quad (4.2)$$

where the repeated sets of upper and lower indices are summed. The representation matrices on  $\mathcal{R}$  of the generators of  $G$  are denoted by  $T_a^{[\mathcal{R}]}$ . The threefold scalar  $\Phi_{\mathcal{R}}^{(k)}$  transforms as  $\mathcal{R}$  under  $G^{\text{diag}}$ .

Next, let us discuss a more general case. Let  $\Phi_{\mathcal{R}_{123}}^{(k)}$  ( $k = 1, 2, 3$ ) be a threefold scalar that belongs to the following representations:

$$\begin{aligned} \Phi_{\mathcal{R}_{123}}^{(1)} &\sim (\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3), & \Phi_{\mathcal{R}_{123}}^{(2)} &\sim (\mathcal{R}_3, \mathcal{R}_1, \mathcal{R}_2), \\ \Phi_{\mathcal{R}_{123}}^{(3)} &\sim (\mathcal{R}_2, \mathcal{R}_3, \mathcal{R}_1). \end{aligned} \quad (4.3)$$

We denote elements of the representation matrices  $T_a^{[\mathcal{R}_k]}$  of the generators by  $(T_a^{[\mathcal{R}_k]})_{\beta_k}^{\alpha_k}$ , where the indices  $\alpha_k$  and  $\beta_k$  run from 1 to  $\dim(\mathcal{R}_k)$ . The component of  $\Phi_{\mathcal{R}_{123}}^{(k)}$  is written as

$$(\Phi_{\mathcal{R}_{123}}^{(1)})_{\alpha_1 \alpha_2 \alpha_3}, \quad (\Phi_{\mathcal{R}_{123}}^{(2)})_{\alpha_3 \alpha_1 \alpha_2}, \quad (\Phi_{\mathcal{R}_{123}}^{(3)})_{\alpha_2 \alpha_3 \alpha_1}. \quad (4.4)$$

We introduce a convenient notations  $\Phi_{\mathcal{R}_{123}}^{(k+3)} \equiv \Phi_{\mathcal{R}_{123}}^{(k)}$  ( $k \in \mathbb{Z}$ ) and  $(\Phi_{\mathcal{R}_{123}}^{(k)})_{[\alpha_1 \alpha_2 \alpha_3]}$ , where the latter represents the components in Eq. (4.4) all at once, that is,  $(\Phi_{\mathcal{R}_{123}}^{(1)})_{[\alpha_1 \alpha_2 \alpha_3]} = (\Phi_{\mathcal{R}_{123}}^{(1)})_{\alpha_1 \alpha_2 \alpha_3}$ ,  $(\Phi_{\mathcal{R}_{123}}^{(2)})_{[\alpha_1 \alpha_2 \alpha_3]} = (\Phi_{\mathcal{R}_{123}}^{(2)})_{\alpha_3 \alpha_1 \alpha_2}$ , and  $(\Phi_{\mathcal{R}_{123}}^{(3)})_{[\alpha_1 \alpha_2 \alpha_3]} = (\Phi_{\mathcal{R}_{123}}^{(3)})_{\alpha_2 \alpha_3 \alpha_1}$ . The  $\mathbb{Z}_3^{(\text{ex})}$  transformation law of the threefold field is defined as

$$(\Phi_{\mathcal{R}_{123}}^{(1)})_{\alpha_1 \alpha_2 \alpha_3} \rightarrow \omega^p (\Phi_{\mathcal{R}_{123}}^{(2)})_{\alpha_3 \alpha_1 \alpha_2}, \quad (4.5)$$

$$(\Phi_{\mathcal{R}_{123}}^{(2)})_{\alpha_3 \alpha_1 \alpha_2} \rightarrow \omega^p (\Phi_{\mathcal{R}_{123}}^{(3)})_{\alpha_2 \alpha_3 \alpha_1}, \quad (4.6)$$

$$(\Phi_{\mathcal{R}_{123}}^{(3)})_{\alpha_2 \alpha_3 \alpha_1} \rightarrow \omega^p (\Phi_{\mathcal{R}_{123}}^{(1)})_{\alpha_1 \alpha_2 \alpha_3}, \quad (4.7)$$

which can be summarized as

$$(\Phi_{\mathcal{R}_{123}}^{(k)})_{[\alpha_1 \alpha_2 \alpha_3]} \rightarrow (\Phi_{\mathcal{R}_{123}}^{(k+1)})_{[\alpha_1 \alpha_2 \alpha_3]}. \quad (4.8)$$



We note that the phase factor  $\omega^p$  appearing in the above can be absorbed by the field redefinitions for the case with complex scalars. The  $\mathbb{Z}_3^{(\text{ex})}$ -invariant kinetic term for  $\Phi_{\mathcal{R}_{123}}^{(k)}$  is given by

$$\begin{aligned} \mathcal{L}(\Phi_{\mathcal{R}_{123}}^{(k)}) &\equiv \sum_{k=1}^3 |D_M^{(k)} \Phi_{\mathcal{R}_{123}}^{(k)}|^2 \\ &= |(D_M^{(1)})_{\alpha_1 \alpha_2 \alpha_3}^{\beta_1 \beta_2 \beta_3} (\Phi_{\mathcal{R}_{123}}^{(1)})_{\beta_1 \beta_2 \beta_3}|^2 \\ &\quad + |(D_M^{(2)})_{\alpha_3 \alpha_1 \alpha_2}^{\beta_3 \beta_1 \beta_2} (\Phi_{\mathcal{R}_{123}}^{(2)})_{\beta_3 \beta_1 \beta_2}|^2 \\ &\quad + |(D_M^{(3)})_{\alpha_2 \alpha_3 \alpha_1}^{\beta_2 \beta_3 \beta_1} (\Phi_{\mathcal{R}_{123}}^{(3)})_{\beta_2 \beta_3 \beta_1}|^2, \end{aligned} \quad (4.9)$$

where the covariant derivatives are written as follows:

$$\begin{aligned} (D_M^{(1)})_{\alpha_1 \alpha_2 \alpha_3}^{\beta_1 \beta_2 \beta_3} &= \delta_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \partial_M + ig \{ A_M^{(1)a} (T_a^{[\mathcal{R}_1]})_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \\ &\quad + \delta_{\alpha_1}^{\beta_1} A_M^{(2)a} (T_a^{[\mathcal{R}_2]})_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \\ &\quad + \delta_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} A_M^{(3)a} (T_a^{[\mathcal{R}_3]})_{\alpha_3}^{\beta_3} \}, \end{aligned} \quad (4.10)$$

$$\begin{aligned} (D_M^{(2)})_{\alpha_3 \alpha_1 \alpha_2}^{\beta_3 \beta_1 \beta_2} &= \delta_{\alpha_3}^{\beta_3} \delta_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \partial_M + ig \{ A_M^{(1)a} (T_a^{[\mathcal{R}_3]})_{\alpha_3}^{\beta_3} \delta_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \\ &\quad + \delta_{\alpha_3}^{\beta_3} A_M^{(2)a} (T_a^{[\mathcal{R}_1]})_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \\ &\quad + \delta_{\alpha_3}^{\beta_3} \delta_{\alpha_1}^{\beta_1} A_M^{(3)a} (T_a^{[\mathcal{R}_2]})_{\alpha_2}^{\beta_2} \}, \end{aligned} \quad (4.11)$$

$$\begin{aligned} (D_M^{(3)})_{\alpha_2 \alpha_3 \alpha_1}^{\beta_2 \beta_3 \beta_1} &= \delta_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \delta_{\alpha_1}^{\beta_1} \partial_M + ig \{ A_M^{(1)a} (T_a^{[\mathcal{R}_2]})_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \delta_{\alpha_1}^{\beta_1} \\ &\quad + \delta_{\alpha_2}^{\beta_2} A_M^{(2)a} (T_a^{[\mathcal{R}_3]})_{\alpha_3}^{\beta_3} \delta_{\alpha_1}^{\beta_1} \\ &\quad + \delta_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} A_M^{(3)a} (T_a^{[\mathcal{R}_1]})_{\alpha_1}^{\beta_1} \}. \end{aligned} \quad (4.12)$$

From the  $\mathbb{Z}_3^{(\text{ex})}$  transformation law of the gauge field,  $A_M^{(k)a} \rightarrow A_M^{(k+1)a}$ , we find that the above covariant derivatives transform as  $(D_M^{(k)})_{[\alpha_1 \alpha_2 \alpha_3]}^{[\beta_1 \beta_2 \beta_3]} \rightarrow (D_M^{(k+1)})_{[\alpha_1 \alpha_2 \alpha_3]}^{[\beta_1 \beta_2 \beta_3]}$ , where we use the same notations for the indices as  $(\Phi_{\mathcal{R}_{123}}^{(k)})_{[\alpha_1 \alpha_2 \alpha_3]}$ . The transformation law helps us to see the  $\mathbb{Z}_3^{(\text{ex})}$  invariance of the above Lagrangian.

Let us discuss the irreducible decomposition of  $\Phi_{\mathcal{R}_{123}}^{(k)}$  under  $G^{\text{diag}}$ . For any  $k$ ,  $\Phi_{\mathcal{R}_{123}}^{(k)}$  transforms under  $G^{\text{diag}}$  as the common reducible direct product representation  $\mathcal{R}_1 \otimes \mathcal{R}_2 \otimes \mathcal{R}_3$ , which can be decomposed into the direct sum of irreducible representations  $\tilde{\mathcal{R}}_i$  ( $i = 1, \dots, n$ ) as

$$\mathcal{R}_1 \otimes \mathcal{R}_2 \otimes \mathcal{R}_3 = \tilde{\mathcal{R}}_1 \oplus \tilde{\mathcal{R}}_2 \oplus \dots \oplus \tilde{\mathcal{R}}_n. \quad (4.13)$$

This ensures that, in the representation space, there exist linear transformations that decompose  $(\Phi_{\mathcal{R}_{123}}^{(k)})_{[\alpha_1 \alpha_2 \alpha_3]}$  into a set of irreducible representations under  $G^{\text{diag}}$  as

$$(\Phi_{\mathcal{R}_{123}}^{(k)})_{[\alpha_1 \alpha_2 \alpha_3]} \rightarrow (\Phi_{\tilde{\mathcal{R}}_1}^{(k)})_{\tilde{\alpha}_1} \oplus (\Phi_{\tilde{\mathcal{R}}_2}^{(k)})_{\tilde{\alpha}_2} \oplus \dots \oplus (\Phi_{\tilde{\mathcal{R}}_n}^{(k)})_{\tilde{\alpha}_n}, \quad (4.14)$$

where  $\tilde{\alpha}_i$  runs from 1 to  $\dim(\tilde{\mathcal{R}}_i)$ .<sup>6</sup> Thus, we can find a basis in the representation space such that each irreducible representation transforms under the  $\mathbb{Z}_3^{(\text{ex})}$  transformation as

$$(\Phi_{\tilde{\mathcal{R}}_i}^{(k)})_{\tilde{\alpha}_i} \xrightarrow{\mathbb{Z}_3^{(\text{ex})}} \omega^p (\Phi_{\tilde{\mathcal{R}}_i}^{(k+1)})_{\tilde{\alpha}_i}. \quad (4.15)$$

The above discussion means that a general threefold scalar transforms under  $G^{\text{diag}}$  as a set of the threefold scalars of the type in Eq. (4.1); this is schematically written as

$$\begin{aligned} &(\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3) + (\mathcal{R}_3, \mathcal{R}_1, \mathcal{R}_2) + (\mathcal{R}_2, \mathcal{R}_3, \mathcal{R}_1) \\ &\sim \sum_{\tilde{\mathcal{R}}_i} [(\tilde{\mathcal{R}}_i, \mathbf{1}, \mathbf{1}) + (\mathbf{1}, \tilde{\mathcal{R}}_i, \mathbf{1}) + (\mathbf{1}, \mathbf{1}, \tilde{\mathcal{R}}_i)]. \end{aligned} \quad (4.16)$$

We should note that the above relation for matter fields is limited for the transformation properties under  $G^{\text{diag}}$ , while the couplings between the matter fields and the Wilson line phases, which belong to  $(G \times G \times G)/G^{\text{diag}}$ , are slightly modified from the above. We will discuss the modification with an explicit example in the next section.

Finally let us discuss the onefold scalar  $\Phi_{\mathcal{R}^3}$ , which belongs to the following representation:

$$\Phi_{\mathcal{R}^3} \sim (\mathcal{R}, \mathcal{R}, \mathcal{R}). \quad (4.17)$$

The component of the onefold is denoted by  $(\Phi_{\mathcal{R}^3})_{\alpha_1 \alpha_2 \alpha_3}$ , which transforms as  $(\Phi_{\mathcal{R}^3})_{\alpha_1 \alpha_2 \alpha_3} \rightarrow \omega^p (\Phi_{\mathcal{R}^3})_{\alpha_3 \alpha_1 \alpha_2}$  under the  $\mathbb{Z}_3^{(\text{ex})}$  transformation. We note that the phase factor  $\omega^p$  cannot be absorbed into field redefinitions in the onefold case. If one considers the threefold scalar of the representation  $\mathcal{R}_1 = \mathcal{R}_2 = \mathcal{R}_3$ , whose  $\mathbb{Z}_3^{(\text{ex})}$  transformation law is given by  $(\Phi_{\mathcal{R}_{123}}^{(k)})_{[\alpha_1 \alpha_2 \alpha_3]} \rightarrow \omega^{p'} (\Phi_{\mathcal{R}_{123}}^{(k+1)})_{[\alpha_1 \alpha_2 \alpha_3]}$ , the linear combination  $\sum_{k=1}^3 \omega^{-(p-p')k} \Phi_{\mathcal{R}_{123}}^{(k)}$  has the same transformation law of the onefold scalar. The kinetic term for the onefold scalar is given by

$$\mathcal{L}(\Phi_{\mathcal{R}^3}) \equiv |(D_M)_{\alpha_1 \alpha_2 \alpha_3}^{\beta_1 \beta_2 \beta_3} (\Phi_{\mathcal{R}^3})_{\beta_1 \beta_2 \beta_3}|^2, \quad (4.18)$$

$$\begin{aligned} (D_M)_{\alpha_1 \alpha_2 \alpha_3}^{\beta_1 \beta_2 \beta_3} &= \delta_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \partial_M \\ &\quad + ig \{ A_M^{(1)a} (T_a^{[\mathcal{R}]})_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} + A_M^{(2)a} \delta_{\alpha_1}^{\beta_1} (T_a^{[\mathcal{R}]})_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \\ &\quad + A_M^{(3)a} \delta_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} (T_a^{[\mathcal{R}]})_{\alpha_3}^{\beta_3} \}, \end{aligned} \quad (4.19)$$

<sup>6</sup>The linear transformations that give Eq. (4.14) generally depend on  $k$  of  $\Phi_{\mathcal{R}_{123}}^{(k)}$ .

where the operator  $(D_M \Phi_{\mathcal{R}^3})_{\alpha_1 \alpha_2 \alpha_3}$  is invariant up to phase factors under the  $\mathbb{Z}_3^{(\text{ex})}$  transformation.

### B. Lagrangian for bulk fermion fields

Let us discuss bulk fermion fields. The notation of the fermion fields in six dimensions is summarized in Appendix D. We denote the 6D Weyl fermion with the positive and negative chiralities by  $\Psi^+$  and  $\Psi^-$ , respectively. Each of the 6D Weyl fermions involves a vectorlike pair of the 4D Weyl fermions,  $\psi_L$  and  $\psi_R$ .

Let  $\Psi_{\mathcal{R}}^{\pm(k)}$  be a  $\mathbb{Z}_3^{(\text{ex})}$  threefold 6D Weyl fermion that belongs to the representation as in Eq. (4.1). Its component is denoted by  $(\Psi_{\mathcal{R}}^{\pm(k)})_{\alpha}$ , where the subscript  $\alpha$  runs from one to  $\dim(\mathcal{R})$ . The  $\mathbb{Z}_3^{(\text{ex})}$  transformation is defined as  $(\Psi_{\mathcal{R}}^{\pm(k)})_{\alpha} \rightarrow \omega^{p^{\pm}} (\Psi_{\mathcal{R}}^{\pm(k+1)})_{\alpha}$ , where  $p^{\pm} \in \{0, \pm 1\}$ . The  $\mathbb{Z}_3^{(\text{ex})}$ -invariant kinetic term is given by

$$\mathcal{L}(\Psi_{\mathcal{R}}^{\pm(k)}) \equiv \sum_{k=1}^3 \overline{(\Psi_{\mathcal{R}}^{\pm(k)})}^{\alpha} i \Gamma^M (D_M^{(k)})_{\alpha}^{\beta} (\Psi_{\mathcal{R}}^{\pm(k)})_{\beta}, \quad (4.20)$$

where  $\Gamma^M$  is the 6D gamma matrix, given in Appendix D. The covariant derivative  $(D_M^{(k)})_{\alpha}^{\beta}$  is the same form as in Eq. (4.2). Using 4D Weyl fermions  $\psi_{\mathcal{R},L}^{\pm(k)}$  and  $\psi_{\mathcal{R},R}^{\pm(k)}$ , we can write

$$\Psi_{\mathcal{R}}^{+(k)} \equiv \begin{pmatrix} \psi_{\mathcal{R},L}^{+(k)} \\ \psi_{\mathcal{R},R}^{+(k)} \end{pmatrix}, \quad \Psi_{\mathcal{R}}^{-(k)} \equiv \begin{pmatrix} \psi_{\mathcal{R},R}^{-(k)} \\ \psi_{\mathcal{R},L}^{-(k)} \end{pmatrix}. \quad (4.21)$$

From Eq. (D22), the Lagrangian can be rewritten by

$$\begin{aligned} \mathcal{L}(\Psi_{\mathcal{R}}^{+(k)}) &= \sum_{k=1}^3 \overline{(\psi_{\mathcal{R},L}^{+(k)}, -\psi_{\mathcal{R},R}^{+(k)})} \begin{pmatrix} i\gamma^{\mu} D_{\mu}^{(k)} & -\tilde{D}_y^{(k)} \\ -\tilde{D}_y^{(k)} & -i\gamma^{\mu} D_{\mu}^{(k)} \end{pmatrix} \\ &\times \begin{pmatrix} \psi_{\mathcal{R},L}^{+(k)} \\ \psi_{\mathcal{R},R}^{+(k)} \end{pmatrix}, \end{aligned} \quad (4.22)$$

$$\begin{aligned} \mathcal{L}(\Psi_{\mathcal{R}}^{-(k)}) &= \sum_{k=1}^3 \overline{(\psi_{\mathcal{R},R}^{-(k)}, -\psi_{\mathcal{R},L}^{-(k)})} \begin{pmatrix} i\gamma^{\mu} D_{\mu}^{(k)} & -\tilde{D}_y^{(k)} \\ -\tilde{D}_y^{(k)} & -i\gamma^{\mu} D_{\mu}^{(k)} \end{pmatrix} \\ &\times \begin{pmatrix} \psi_{\mathcal{R},R}^{-(k)} \\ \psi_{\mathcal{R},L}^{-(k)} \end{pmatrix}, \end{aligned} \quad (4.23)$$

where we have defined

$$\begin{aligned} \tilde{D}_y^{(k)} &= \frac{2}{3} (D_{y^1}^{(k)} + \omega D_{y^2}^{(k)} + \bar{\omega} D_{y^3}^{(k)}), \\ \bar{\tilde{D}}_y^{(k)} &= \frac{2}{3} (D_{y^1}^{(k)} + \bar{\omega} D_{y^2}^{(k)} + \omega D_{y^3}^{(k)}), \end{aligned} \quad (4.24)$$

and the indices in the representation space of  $\mathcal{R}$  are suppressed.

For a general threefold fermion, denoted by  $\Psi_{\mathcal{R}_{123}}^{\pm(k)}$ , whose representation is  $\mathcal{R}_1 \otimes \mathcal{R}_2 \otimes \mathcal{R}_3$ , we can write the Lagrangian by using the covariant derivatives of the forms in Eqs. (4.10)–(4.12). The irreducible decomposition under  $G^{\text{diag}}$  is obtained as the scalar case, discussed in the previous subsection.

Let us turn to deal with the onefold 6D Weyl fermions, which is denoted by  $\Psi_{\mathcal{R}^3}^{\pm}$ . Let  $(\Psi_{\mathcal{R}^3}^{\pm})_{\alpha_1 \alpha_2 \alpha_3}$  be a component of  $\Psi_{\mathcal{R}^3}^{\pm}$ , which is defined to transform into  $(\Psi_{\mathcal{R}^3}^{\pm})_{\alpha_3 \alpha_1 \alpha_2}$  under the  $\mathbb{Z}_3^{(\text{ex})}$  transformation. The Lagrangian is written by

$$\mathcal{L}(\Psi_{\mathcal{R}^3}^{\pm}) = \overline{(\Psi_{\mathcal{R}^3}^{\pm})}^{\alpha_1 \alpha_2 \alpha_3} i \Gamma^M (D_M)^{\beta_1 \beta_2 \beta_3}_{\alpha_1 \alpha_2 \alpha_3} (\Psi_{\mathcal{R}^3}^{\pm})_{\beta_1 \beta_2 \beta_3}, \quad (4.25)$$

where the covariant derivative is the same as in Eq. (4.18). Using 4D Weyl fermions  $\psi_{\mathcal{R}^3,L}^{\pm}$  and  $\psi_{\mathcal{R}^3,R}^{\pm}$ , we can write

$$\Psi_{\mathcal{R}^3}^{+} \equiv \begin{pmatrix} \psi_{\mathcal{R}^3,L}^{+} \\ \psi_{\mathcal{R}^3,R}^{+} \end{pmatrix}, \quad \Psi_{\mathcal{R}^3}^{-} \equiv \begin{pmatrix} \psi_{\mathcal{R}^3,R}^{-} \\ \psi_{\mathcal{R}^3,L}^{-} \end{pmatrix}. \quad (4.26)$$

Then the Lagrangian can be written as

$$\mathcal{L}(\Psi_{\mathcal{R}^3}^{+}) = \sum_{k=1}^3 \overline{(\psi_{\mathcal{R}^3,L}^{+}, -\psi_{\mathcal{R}^3,R}^{+})} \begin{pmatrix} i\gamma^{\mu} D_{\mu} & -\bar{\tilde{D}}_y \\ -\tilde{D}_y & -i\gamma^{\mu} D_{\mu} \end{pmatrix} \begin{pmatrix} \psi_{\mathcal{R}^3,L}^{+} \\ \psi_{\mathcal{R}^3,R}^{+} \end{pmatrix}, \quad (4.27)$$

$$\mathcal{L}(\Psi_{\mathcal{R}^3}^{-}) = \sum_{k=1}^3 \overline{(\psi_{\mathcal{R}^3,R}^{-}, -\psi_{\mathcal{R}^3,L}^{-})} \begin{pmatrix} i\gamma^{\mu} D_{\mu} & -\bar{\tilde{D}}_y \\ -\tilde{D}_y & -i\gamma^{\mu} D_{\mu} \end{pmatrix} \begin{pmatrix} \psi_{\mathcal{R}^3,R}^{-} \\ \psi_{\mathcal{R}^3,L}^{-} \end{pmatrix}, \quad (4.28)$$

where  $\tilde{D}_y$  and  $\bar{\tilde{D}}_y$  are defined as Eq. (4.24) with the covariant derivative in Eq. (4.18), and the indices in the representation space are suppressed here.

In general, bulk gauge anomalies arise from 6D chiral fermions. The requirement of cancellations of the anomalies gives constraints on the matter contents of theories [21,22,29,30]. In our setup, bulk anomaly cancellations can be ensured by introducing vectorlike sets of 6D Weyl fermions. There also appear 4D gauge anomalies on the boundaries, i.e., the fixed points on  $T^2/\mathbb{Z}_3$ . Such 4D anomalies depend on BCs for fermions and will be discussed in the next subsection.

### C. ORBIFOLD BOUNDARY CONDITIONS AND LOW-ENERGY MASS SPECTRA

We here discuss the BCs for matter fields. First, let us see the transformation laws of covariant derivatives under  $\hat{T}_1$  and  $\hat{S}_0$ , which must be consistent with the BCs for gauge fields. From Eqs. (3.7) and (3.8), we find that the covariant

derivatives in Eqs. (4.2) and (4.10)–(4.12) for threefolds and in Eq. (4.18) for onefolds transform as

$$\hat{T}_1[(D_{\{\mu,y^i\}}^{(k)})_{\alpha}^{\beta}] = (D_{\{\mu,y^i\}}^{(k)})_{\alpha}^{\beta}, \quad \hat{S}_0[(D_{\{\mu,y^i\}}^{(k)})_{\alpha}^{\beta}] = (D_{\{\mu,y^{i-1}\}}^{(k+1)})_{\alpha}^{\beta}, \quad (4.29)$$

$$\begin{aligned} \hat{T}_1[(D_{\{\mu,y^i\}}^{(k)})_{[\alpha_1\alpha_2\alpha_3]}^{[\beta_1\beta_2\beta_3]}] &= (D_{\{\mu,y^i\}}^{(k)})_{[\alpha_1\alpha_2\alpha_3]}^{[\beta_1\beta_2\beta_3]}, \\ \hat{S}_0[(D_{\{\mu,y^i\}}^{(k)})_{[\alpha_1\alpha_2\alpha_3]}^{[\beta_1\beta_2\beta_3]}] &= (D_{\{\mu,y^{i-1}\}}^{(k+1)})_{[\alpha_1\alpha_2\alpha_3]}^{[\beta_1\beta_2\beta_3]}, \end{aligned} \quad (4.30)$$

$$\begin{aligned} \hat{T}_1[(D_{\{\mu,y^i\}})_{\alpha_1\alpha_2\alpha_3}^{\beta_1\beta_2\beta_3}] &= (D_{\{\mu,y^i\}})_{\alpha_1\alpha_2\alpha_3}^{\beta_1\beta_2\beta_3}, \\ \hat{S}_0[(D_{\{\mu,y^i\}})_{\alpha_1\alpha_2\alpha_3}^{\beta_1\beta_2\beta_3}] &= (D_{\{\mu,y^{i-1}\}})_{\alpha_3\alpha_1\alpha_2}^{\beta_3\beta_1\beta_2}, \end{aligned} \quad (4.31)$$

where we have used the shorthand notation to show the boundary conditions for the covariant derivative along  $x^\mu$  and  $y^i$  by the subscript  $\{\mu, y^i\}$ .

The BCs for the matter fields are taken to be consistent with the above transformations and written as

$$\begin{aligned} \phi(x^\mu, \hat{T}_1[y^i]) &= \omega^{p_i} \phi(x^\mu, y^i), \\ \phi(x^\mu, \hat{S}_0[y^i]) &= \omega^{p_s} \phi_S(x^\mu, y^i), \end{aligned} \quad (4.32)$$

where a pair of fields  $\phi$  and  $\phi_S$  represent the scalars  $\Phi$  and 6D Weyl fermions  $\Psi^\pm$ :

$$\begin{aligned} (\phi, \phi_S) \in & \{((\Phi_{\mathcal{R}}^{(k)})_{\alpha}, (\Phi_{\mathcal{R}}^{(k+1)})_{\alpha}), ((\Phi_{\mathcal{R}_{123}}^{(k)})_{[\alpha_1\alpha_2\alpha_3]}, (\Phi_{\mathcal{R}_{123}}^{(k+1)})_{[\alpha_1\alpha_2\alpha_3]}), \\ & ((\Phi_{\mathcal{R}^3}^{(k)})_{\alpha_1\alpha_2\alpha_3}, (\Phi_{\mathcal{R}^3}^{(k+1)})_{\alpha_1\alpha_2\alpha_3}), ((\Psi_{\mathcal{R}}^{\pm(k)})_{\alpha}, -\tilde{S}_{\Psi}(\Psi_{\mathcal{R}}^{\pm(k+1)})_{\alpha}), \\ & ((\Psi_{\mathcal{R}_{123}}^{\pm(k)})_{[\alpha_1\alpha_2\alpha_3]}, -\tilde{S}_{\Psi}(\Psi_{\mathcal{R}_{123}}^{\pm(k+1)})_{[\alpha_1\alpha_2\alpha_3]}), ((\Psi_{\mathcal{R}^3}^{\pm(k)})_{\alpha_1\alpha_2\alpha_3}, -\tilde{S}_{\Psi}(\Psi_{\mathcal{R}^3}^{\pm(k+1)})_{\alpha_3\alpha_1\alpha_2})\}. \end{aligned} \quad (4.33)$$

The definition of  $\tilde{S}_{\Psi}$  is shown in Eq. (D24), and  $p_i, p_s \in \{0, \pm 1\}$  are chosen by hand for each field. Since the 6D Weyl fermions compose of 4D Weyl fermions, the last three pairs in Eq. (4.33) are rearranged to the six pairs of the 4D Weyl fermions as

$$((\Psi_{\mathcal{R},L}^{\pm(k)})_{\alpha}, \omega^{\pm 1}(\Psi_{\mathcal{R},L}^{\pm(k+1)})_{\alpha}), \quad ((\Psi_{\mathcal{R},R}^{\pm(k)})_{\alpha}, \omega^{\mp 1}(\Psi_{\mathcal{R},R}^{\pm(k+1)})_{\alpha}), \quad (4.34)$$

$$\begin{aligned} ((\Psi_{\mathcal{R}_{123},L}^{\pm(k)})_{[\alpha_1\alpha_2\alpha_3]}, \omega^{\pm 1}(\Psi_{\mathcal{R}_{123},L}^{\pm(k+1)})_{[\alpha_1\alpha_2\alpha_3]}), \\ ((\Psi_{\mathcal{R}_{123},R}^{\pm(k)})_{[\alpha_1\alpha_2\alpha_3]}, \omega^{\mp 1}(\Psi_{\mathcal{R}_{123},R}^{\pm(k+1)})_{[\alpha_1\alpha_2\alpha_3]}), \end{aligned} \quad (4.35)$$

$$\begin{aligned} ((\Psi_{\mathcal{R}^3,L}^{\pm(k)})_{\alpha_1\alpha_2\alpha_3}, \omega^{\pm 1}(\Psi_{\mathcal{R}^3,L}^{\pm(k+1)})_{\alpha_3\alpha_1\alpha_2}), \\ ((\Psi_{\mathcal{R}^3,R}^{\pm(k)})_{\alpha_1\alpha_2\alpha_3}, \omega^{\mp 1}(\Psi_{\mathcal{R}^3,R}^{\pm(k+1)})_{\alpha_3\alpha_1\alpha_2}). \end{aligned} \quad (4.36)$$

Any BCs given above are formally written as

$$\begin{aligned} \phi^{(k)}(x^\mu, \hat{T}_1[y^i]) &= \omega^{p_i} \phi^{(k)}(x^\mu, y^i), \\ \phi^{(k)}(x^\mu, \hat{S}_0[y^i]) &= \omega^{\bar{p}_s} \phi^{(k+1)}(x^\mu, y^i), \end{aligned} \quad (4.37)$$

where  $\phi^{(k+3)} = \phi^{(k)}$  ( $k \in \mathbb{Z}$ ) is a boson or a 4D Weyl fermion and is a component of an irreducible representation under  $G \times G \times G$ . The integer  $\bar{p}_s$  is equal to  $p_s$  for a boson and equal to  $p_s \pm 1$  ( $p_s \mp 1$ ) for a left-handed (right-handed) fermion with the 6D chirality  $\pm$ . In most cases, components in a set  $\{\phi^{(1)}, \phi^{(2)}, \phi^{(3)}\}$  are not identical and are mixed by the  $\mathbb{Z}_3^{(\text{ex})}$  transformation; in this case we call  $\phi^{(k)}$  as a  $\mathbb{Z}_3^{(\text{ex})}$  triplet. There is a special case, where

$\phi^{(k+1)} = \phi^{(k)}$  holds; in this case the field  $\phi^{(k)}$  is an eigenstate of the  $\mathbb{Z}_3^{(\text{ex})}$  transformation and called a  $\mathbb{Z}_3^{(\text{ex})}$  singlet. We list the sets of the form  $\{\phi^{(1)}, \phi^{(2)}, \phi^{(3)}\}$  as follows:

$$\{(\Phi_{\mathcal{R}}^{(1)})_{\alpha}, (\Phi_{\mathcal{R}}^{(2)})_{\alpha}, (\Phi_{\mathcal{R}}^{(3)})_{\alpha}\}, \quad (4.38)$$

$$\{(\Phi_{\mathcal{R}_{123}}^{(1)})_{\alpha_1\alpha_2\alpha_3}, (\Phi_{\mathcal{R}_{123}}^{(2)})_{\alpha_3\alpha_1\alpha_2}, (\Phi_{\mathcal{R}_{123}}^{(3)})_{\alpha_2\alpha_3\alpha_1}\}, \quad (4.39)$$

$$\{(\Phi_{\mathcal{R}^3}^{(1)})_{\alpha_1\alpha_2\alpha_3}, (\Phi_{\mathcal{R}^3}^{(2)})_{\alpha_3\alpha_1\alpha_2}, (\Phi_{\mathcal{R}^3}^{(3)})_{\alpha_2\alpha_3\alpha_1}\}, \quad (4.40)$$

$$\{(\Psi_{\mathcal{R},\{L,R\}}^{\pm(1)})_{\alpha}, (\Psi_{\mathcal{R},\{L,R\}}^{\pm(2)})_{\alpha}, (\Psi_{\mathcal{R},\{L,R\}}^{\pm(3)})_{\alpha}\}, \quad (4.41)$$

$$\{(\Psi_{\mathcal{R}_{123},\{L,R\}}^{\pm(1)})_{\alpha_1\alpha_2\alpha_3}, (\Psi_{\mathcal{R}_{123},\{L,R\}}^{\pm(2)})_{\alpha_3\alpha_1\alpha_2}, (\Psi_{\mathcal{R}_{123},\{L,R\}}^{\pm(3)})_{\alpha_2\alpha_3\alpha_1}\}, \quad (4.42)$$

$$\{(\Psi_{\mathcal{R}^3,\{L,R\}}^{\pm(1)})_{\alpha_1\alpha_2\alpha_3}, (\Psi_{\mathcal{R}^3,\{L,R\}}^{\pm(2)})_{\alpha_3\alpha_1\alpha_2}, (\Psi_{\mathcal{R}^3,\{L,R\}}^{\pm(3)})_{\alpha_2\alpha_3\alpha_1}\}. \quad (4.43)$$

Among them, only the onefold components with  $\alpha_1 = \alpha_2 = \alpha_3$  form  $\mathbb{Z}_3^{(\text{ex})}$  singlets, and the others are  $\mathbb{Z}_3^{(\text{ex})}$  triplets.

Although  $\mathbb{Z}_3^{(\text{ex})}$  singlets are eigenstates of the BCs, triplets are not. From a  $\mathbb{Z}_3^{(\text{ex})}$  triplet, we can define three eigenstates of the BCs, denoted by  $\phi^{[p]}$  ( $p = 0, \pm 1$ ), as

$$\phi^{[p]} = \frac{1}{\sqrt{3}} \sum_{k=1}^3 \omega^{-kp} \phi^{(k)}, \quad \phi^{(k)} = \frac{1}{\sqrt{3}} \sum_{p=-1}^1 \omega^{kp} \phi^{[p]}. \quad (4.44)$$

Then,  $\phi^{[p]}$  obeys the following BCs:

$$\begin{aligned}\phi^{[p]}(x^\mu, \hat{T}_1[y^i]) &= \omega^{p_i} \phi^{[p]}(x^\mu, y^i), \\ \phi^{[p]}(x^\mu, \hat{S}_0[y^i]) &= \omega^{p+\tilde{p}_s} \phi^{[p]}(x^\mu, y^i).\end{aligned}\quad (4.45)$$

We note that  $\phi^{[p]}$  is convenient to examine the KK expansions, which are summarized in Appendix A, while the couplings between matter fields and the Wilson line phases are simplified for  $\phi^{(k)}$ .

From the eigenvalues of the BCs, we can find zero modes, which are constant excitations over the extradimensional space. The zero mode can appear as a light degree of freedom in a low-energy effective 4D theory, where gauge symmetry  $G \times G \times G$  is reduced to  $G^{\text{diag}}$  as discussed in Sec. III B. In contrast, the other modes have  $\mathcal{O}(1/R)$  masses and become heavy. For  $\mathbb{Z}_3^{(\text{ex})}$  triplets,  $\phi^{[p]}$  with  $p_t = p + \tilde{p}_s = 0$  in Eq. (4.45) has a zero mode. For  $\mathbb{Z}_3^{(\text{ex})}$  singlets, fields with  $p_t = \tilde{p}_s = 0$  have zero modes. Note that fields with  $p_t = \pm 1$  do not have any zero modes.

We discuss zero mode spectrum that arises from threefold fields in detail. Since threefold fields do not involve any  $\mathbb{Z}_3^{(\text{ex})}$  singlet, they are always organized into  $\mathbb{Z}_3^{(\text{ex})}$  triplets. For the case with a threefold scalar  $\Phi_{\mathcal{R}}^{(k)}$  with  $p_t = 0$ , there appear zero modes, contained in the triplet component  $\phi^{[-p_s]}$ . These zero modes belong to the representation  $\mathcal{R}$  under  $G^{\text{diag}}$ . For the fermion case, a threefold  $\Psi_{\mathcal{R}}^{\pm(k)}$  can be decomposed into  $\psi_{\mathcal{R},L}^{\pm(k)} + \psi_{\mathcal{R},R}^{\pm(k)}$ . For the case with a  $\Psi_{\mathcal{R}}^{+(k)}$  ( $\Psi_{\mathcal{R}}^{-(k)}$ ) having  $p_t = 0$ , a vectorlike pair  $\psi_{\mathcal{R},L}^{+(k)}$

and  $\psi_{\mathcal{R},R}^{+(k)}$  ( $\psi_{\mathcal{R},R}^{-(k)}$  and  $\psi_{\mathcal{R},L}^{-(k)}$ ) has vectorlike zero modes, which appear from the triplet components  $\phi^{[-p_s-1]}$  and  $\phi^{[-p_s+1]}$ , respectively. Thus, in these cases we always have vectorlike fermion zero modes, which belongs to  $\mathcal{R}$  under  $G^{\text{diag}}$ . Similar discussions hold also for a more general threefold scalar  $\Phi_{\mathcal{R}_{123}}^{(k)}$  and fermion  $\Psi_{\mathcal{R}_{123}}^{\pm(k)}$ .

Next, we discuss zero mode spectrum of onefold fields. A onefold involves both  $\mathbb{Z}_3^{(\text{ex})}$  singlets and triplets except for the case with the trivial representation  $\mathcal{R} = \mathbf{1}$ . From  $\mathbb{Z}_3^{(\text{ex})}$  singlets in a onefold scalar  $\Phi_{\mathcal{R}^3}$  with  $p_t = 0$ , zero modes appear only if  $p_s = 0$ . For  $\mathbb{Z}_3^{(\text{ex})}$  triplets in  $\Phi_{\mathcal{R}^3}$  with  $p_t = 0$ , zero modes appear from the component  $\phi^{[-p_s]}$ . For the fermion case, both  $\psi_{\mathcal{R}^3,L}^{\pm}$  and  $\psi_{\mathcal{R}^3,R}^{\pm}$  in a onefold  $\Psi_{\mathcal{R}^3}^{\pm}$  have  $\mathbb{Z}_3^{(\text{ex})}$  singlets. For the case with  $p_t = 0$ , singlets in  $\psi_{\mathcal{R}^3,L}^{\pm}$  ( $\psi_{\mathcal{R}^3,R}^{\pm}$ ) have zero modes only if  $p_s = -1$  ( $p_s = 1$ ). These zero modes of  $\mathbb{Z}_3^{(\text{ex})}$  singlets yield chiral fermion mass spectrum. There also exist triplets in  $\Psi_{\mathcal{R}^3}^{\pm}$ . For  $p_t = 0$ , zero modes appear from the triplet components  $\phi^{[-p_s \mp 1]}$  ( $\phi^{[-p_s \pm 1]}$ ), constructed from  $\psi_{\mathcal{R}^3,L}^{\pm}$  ( $\psi_{\mathcal{R}^3,R}^{\pm}$ ). The zero modes of  $\mathbb{Z}_3^{(\text{ex})}$  triplets always compose vectorlike pairs of 4D fermions. We note that any zero modes belong to irreducible representations, which are contained in the irreducible decomposition of  $\mathcal{R} \otimes \mathcal{R} \otimes \mathcal{R}$  under  $G^{\text{diag}}$ .

As an illustrative example, we consider  $G = SU(N)$  and the  $N$ -dimensional fundamental representation as  $\mathcal{R}$ . In this case, the irreducible decomposition of  $\mathcal{R} \otimes \mathcal{R} \otimes \mathcal{R}$  is shown by the following Young tableaux:

$$\square \otimes \square \otimes \square = \square\square\square \oplus 2 \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array} \oplus \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \end{array}. \quad (4.46)$$

One sees that  $\mathbb{Z}_3^{(\text{ex})}$  singlets in  $\Phi_{\mathcal{R}^3}$  and  $\Psi_{\mathcal{R}^3}^{\pm}$  always belong to the first representation on the right-hand side of Eq. (4.46). These singlets carry  $N$  out of  $N^3$  degrees of freedom, and the rest  $N^3 - N$  degrees of freedom form  $(N^3 - N)/3 = N(N-1)(N+1)/3$  triplets. For  $p_t = p_s = 0$ , since the  $\mathbb{Z}_3^{(\text{ex})}$  singlets have zero modes, there appear  $N + (N^3 - N)/3$  degrees of freedom appear as

zero modes, whose representations correspond to the first and third terms on the right-hand side of Eq. (4.46). On the other hand, for  $p_s = \pm 1$  case with  $p_t = 0$ , there appear  $(N^3 - N)/3$  degrees of freedom as zero modes, which transform as the representation corresponds to the second terms on the right-hand side of Eq. (4.46). Consistently to the above, one sees the relation

$$\begin{aligned}\# \left( \square\square\square \oplus \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \end{array} \right) - \# \left( \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array} \right) &= \left( \frac{N}{6}(N+1)(N+2) + \frac{N}{6}(N-1)(N-2) \right) - \frac{N}{3}(N^2-1) \\ &= N,\end{aligned}\quad (4.47)$$

where  $\sharp(*)$  is the degrees of freedom of  $*$ . We see that  $N$  in Eq. (4.47) corresponds to the degrees of freedom of  $\mathbb{Z}_3^{(\text{ex})}$  singlet components.

Let us examine the fermion zero modes in the  $SU(N)$  case. For the case with onefold fermions, zero mode spectrum can become chiral. For example, we consider the case with a onefold  $\Psi_{\mathcal{R}^3}^+$  of  $p_t = 0$ . In this case, the representations of the zero modes depend on  $p_s$ , which are summarized as follows:

$$p_s = 0 \quad : \quad (\psi_{\mathcal{R}^3,L}^+)_{\text{zero mode}} \sim \begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array}, \quad (\psi_{\mathcal{R}^3,R}^+)_{\text{zero mode}} \sim \begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array}, \quad (4.48)$$

$$p_s = 1 \quad : \quad (\psi_{\mathcal{R}^3,L}^+)_{\text{zero mode}} \sim \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array}, \quad (\psi_{\mathcal{R}^3,R}^+)_{\text{zero mode}} \sim \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \end{array} \oplus \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array}, \quad (4.49)$$

$$p_s = -1 \quad : \quad (\psi_{\mathcal{R}^3,L}^+)_{\text{zero mode}} \sim \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \end{array} \oplus \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array}, \quad (\psi_{\mathcal{R}^3,R}^+)_{\text{zero mode}} \sim \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array}. \quad (4.50)$$

Thus, low-energy spectrum of 4D fermions is chiral for  $p_s = \pm 1$ , but vectorlike for  $p_s = 0$ . A similar discussion holds for the case with  $\Psi_{\mathcal{R}^3}^-$ .

Finally, we give comments on 4D gauge anomalies. If there are fermion zero modes, they generally contribute to the anomalies. For threefold fermions, their zero modes are always vector-like and do not give 4D anomalies. On the other hand, onefold fermions can have chiral zero modes and thus generally generate 4D anomalies. Thus, a requirement of the cancellation of 4D anomalies constrains the onefold fermion contents. In addition to the zero mode anomalies, localized anomalies induced at the fixed points  $y_{f(r)}^i$  ( $r = 0, 1, 2$ ), defined in Eq. (2.12), should also be concerned [22]. The localized contributions arise even if the fermion has  $p_t = \pm 1$ , in which case there is no zero modes. In our setup, contribution to the localized anomalies at  $y_{f(r)}^i$  can arise from a fermion  $\psi(x^\mu, y^i)$  that satisfy the BCs  $\psi(x^\mu, \hat{\mathcal{S}}_r[y^i]) = \psi(x^\mu, y^i)$ . One can see that the contributions to the localized anomalies at each fixed point from threefold fermions always cancel out since the contributions are always vectorlike. For the onefold fermion, localized anomalies generally exist; it gives constraints on the matter content of the theory. When the localized anomalies vanish, also the 4D anomalies do. Conversely, the 4D anomaly cancellation does not ensure vanishing localized anomalies.

## V. ONE-LOOP EFFECTIVE POTENTIALS FOR WILSON LINE PHASES IN $SU(5)$ MODELS

In this section, we study one-loop effective potentials for the classical background VEVs  $\tilde{a}_{k+\ell}^a$  in Eq. (3.20), which are

related to the Wilson line phase degrees of freedom. As a concrete example, we focus on the case with  $G = SU(5)$ . The discussion can be generalized to other gauge group cases.

### A. Contributions from $\mathbb{Z}_3^{(\text{ex})}$ threefold fields

First, we derive one-loop contributions from a  $\mathbb{Z}_3^{(\text{ex})}$  threefold scalar field to the effective potential. The simplest example is the threefold  $\Phi_5^{(k)}$ , which transforms under  $SU(5) \times SU(5) \times SU(5)$  as

$$\Phi_5^{(1)} \sim (\mathbf{5}, \mathbf{1}, \mathbf{1}), \quad \Phi_5^{(2)} \sim (\mathbf{1}, \mathbf{5}, \mathbf{1}), \quad \Phi_5^{(3)} \sim (\mathbf{1}, \mathbf{1}, \mathbf{5}), \quad (5.1)$$

where  $\mathbf{5}$  and  $\mathbf{1}$  are the fundamental and the trivial representations of  $SU(5)$ , respectively. Based on the discussion in the previous section, we define BCs for their components,  $(\Phi_5^{(k)})_\alpha$  ( $\alpha = 1, \dots, 5$ ), as

$$\begin{aligned} (\Phi_5^{(k)})_\alpha(x^\mu, \hat{\mathcal{T}}_1[y^i]) &= \omega^{p_t} (\Phi_5^{(k)})_\alpha(x^\mu, y^i), \\ (\Phi_5^{(k)})_\alpha(x^\mu, \hat{\mathcal{S}}_0[y^i]) &= \omega^{p_s} (\Phi_5^{(k+1)})_\alpha(x^\mu, y^i). \end{aligned} \quad (5.2)$$

In the following, the fundamental representation of the  $SU(5)$  generators is denoted by  $(T_a^{[5]})_\alpha^\beta \equiv (T_a)_\alpha^\beta$ . From Eq. (4.2), Lagrangian for  $\Phi_5^{(k)}$  has the  $\mathbb{Z}_3^{(\text{ex})}$ -invariant form,

$$\mathcal{L}(\Phi_5^{(k)}) = \sum_{k=1}^3 |(D_M^{(k)})^\beta_\alpha(\Phi_5^{(k)})_\beta|^2, \quad (D_M^{(k)})^\beta_\alpha = \delta^\beta_\alpha \partial_M + ig A_M^{(k)\alpha} (T_a)^\beta_\alpha. \quad (5.3)$$

To obtain the effective potential for  $\tilde{a}_{k+\ell}^\alpha$  in Eq. (3.20), let us expand the Lagrangian in Eq. (5.3) around the classical background VEVs and extract quadratic terms of the quantum fluctuations. As discussed in Sec. III C, we always take a basis where the Wilson line phases are diagonal and have the form like Eq. (3.28). One-loop corrections to the effective potential for the phases can be derived through path integral over the fluctuation  $(\Phi_5^{(k)})_\alpha$ . The quadratic terms are written as follows:

$$\mathcal{L}^{(2)}(\Phi_5^{(k)}) \equiv - \sum_{k=1}^3 (\Phi_5^{(k)\dagger})^\alpha (\delta^\beta_\alpha \square - g^{ij} \langle D_{y^i}^{(k)} \rangle_{\alpha'} \langle D_{y^j}^{(k)} \rangle_{\alpha'}) \times (\Phi_5^{(k)})_\beta, \quad (5.4)$$

$$\langle D_{y^i}^{(k)} \rangle_{\alpha}^\beta \equiv \delta^\beta_\alpha \partial_{y^i} + i \frac{2}{R} \tilde{a}_{i+k}^{\hat{a}} (H_{\hat{a}})^\beta_\alpha, \quad (5.5)$$

where we have defined  $\langle D_{y^i}^{(k)} \rangle_{\alpha}^\beta$  as a background covariant derivative and  $\square = \partial_\mu \partial^\mu$ . The matrices  $H_{\hat{a}}$  ( $\hat{a} = 1, \dots, 4$ ) are the fundamental representation of the Cartan generators of  $SU(5)$ , which we can take as

$$H_1 = \frac{1}{2} \text{diag}(1, 0, 0, 0, -1), \quad H_2 = \frac{1}{2} \text{diag}(0, 1, 0, 0, -1), \\ H_3 = \frac{1}{2} \text{diag}(0, 0, 1, 0, -1), \quad H_4 = \frac{1}{2} \text{diag}(0, 0, 0, 1, -1). \quad (5.6)$$

Thus, the Wilson line phases in Eq. (5.5) are written as

$$2\tilde{a}_{i+k}^{\hat{a}} H_{\hat{a}} = \text{diag}(\tilde{a}_{i+k}^1, \tilde{a}_{i+k}^2, \tilde{a}_{i+k}^3, \tilde{a}_{i+k}^4, \tilde{a}_{i+k}^5), \quad \text{where} \\ \tilde{a}_{i+k}^5 = - \sum_{\hat{a}=1}^4 \tilde{a}_{i+k}^{\hat{a}}. \quad (5.7)$$

We now readily rewrite the quadratic Lagrangian in Eq. (5.4) as

$$\mathcal{L}^{(2)}(\Phi_5^{(k)}) = - \sum_{\alpha=1}^5 \sum_{k=1}^3 (\Phi_5^{(k)\dagger})^\alpha (\square + \hat{M}_{k,\alpha}^2) (\Phi_5^{(k)})_\alpha, \quad (5.8)$$

where we have introduced the differential operator  $\hat{M}_{k,\alpha}^2$  as

$$\hat{M}_{k,\alpha}^2 \equiv g^{ij} \left( -i\partial_{y^i} + \frac{\tilde{a}_{i+k}^\alpha}{R} \right) \left( -i\partial_{y^j} + \frac{\tilde{a}_{j+k}^\alpha}{R} \right) \\ = \frac{2}{3} \sum_{\ell=1}^3 \left( -i\partial_{y^\ell} + \frac{\tilde{a}_{k+\ell}^\alpha}{R} \right)^2. \quad (5.9)$$

We note that the above corresponds to the operator in Eq. (A38).

Based on the discussion in Sec. IV A and the BCs in Eq. (5.2), we see that the components  $\{(\Phi_5^{(1)})_\alpha, (\Phi_5^{(2)})_\alpha, (\Phi_5^{(3)})_\alpha\}$  form a  $\mathbb{Z}_3^{(\text{ex})}$  triplet. In Appendix A, we first show the KK expansion of  $\mathbb{Z}_3^{(\text{ex})}$  singlets in Eq. (A18), and using it, we derive the expansion of triplets in Eq. (A35). Here we briefly provide the overview of the derivation. From the triplet  $\phi^{(k)}$  that obeys the BCs in Eq. (4.37), we can define  $\phi^{[p]}$  that are eigenstates of the BCs as in Eq. (4.45). The KK expansion of  $\phi^{[p]}$  yields the corresponding KK modes  $\tilde{\phi}_{N_1, N_2}^{[p]}$  in Eq. (A30), where  $N_i = n_i + p_i/3$  and  $n_i \in \mathbb{Z}$ . From  $\tilde{\phi}_{N_1, N_2}^{[p]}$ , we can define  $\tilde{\phi}_{N_1, N_2}^{(k)}$  appearing in Eq. (A35). Their KK masses are given by replacing the operator  $-i\partial_{y^\ell}$  in Eq. (5.9) by  $N_\ell/R$  ( $N_3 = -N_1 - N_2$ ). In the present case, the KK masses for  $(\Phi_5^{(k)})_\alpha$  are given by

$$M_{k,\alpha}^2 = \frac{2}{3R^2} \sum_{\ell=1}^3 (N_\ell + \tilde{a}_{\ell+k}^\alpha)^2, \quad \text{where} \\ N_i = n_i + p_i/3, \quad N_3 = -N_1 - N_2. \quad (5.10)$$

For details, please refer to Appendix A.

With the above result, the 4D effective Lagrangian in Eq. (5.4) is rewritten by KK modes of the triplet, and we can integrate them to obtain the effective potential. The derivation of the potential is shown in Appendix B. Using the result shown in Eq. (B14), we find that the effective potential contribution from a real degree of freedom in  $(\Phi_5^{(k)})_\alpha$  is given by

$$\mathcal{V}^{(p_i)}(\tilde{a}_i^\alpha) = - \frac{\sqrt{3}}{32\pi^7 R^4} \sum_{w^1, w^2 \in \mathbb{Z}'} \frac{\cos(2\pi[w^1(p_i/3 + \tilde{a}_1^\alpha) + w^2(p_i/3 + \tilde{a}_2^\alpha)])}{[(w^1)^2 - w^1 w^2 + (w^2)^2]^3}, \quad (5.11)$$

where we have used  $\tilde{a}_i^\alpha$  ( $i = 1, 2$ ) as the parameter of the potential since they are taken to be the independent variables among  $\tilde{a}_\ell^\alpha$  ( $\ell = 1, 2, 3$ ). As discussed in Appendix B, the summation with respect to  $w^1$  and  $w^2$  is taken over for all integers except for  $(w^1, w^2) = (0, 0)$ , which is denoted by  $w^1, w^2 \in \mathbb{Z}'$ . We note that the potential in Eq. (5.11) can also be naturally expressed by the vector notation as

$$\mathcal{V}^{(p_i)}(\tilde{a}_i^\alpha) = -\frac{\sqrt{3}}{32\pi^7 R^4} \sum_{\mathbf{w} \in \Lambda'_w} \frac{\cos(2\pi \mathbf{w} \cdot \tilde{\mathbf{a}}^{\alpha'})}{(|\mathbf{w}|^2)^3}, \quad (5.12)$$

where we have introduced the vector  $\mathbf{w}$  and the lattice  $\Lambda'_w$  as

$$\Lambda'_w = \{\mathbf{w} = w^1 \mathbf{e}_1 + w^2 \mathbf{e}_2 | w^1, w^2 \in \mathbb{Z}'\}, \quad (5.13)$$

and the dual vector  $\tilde{\mathbf{a}}^{\alpha'} = (p_i/3 + \tilde{a}_1^\alpha) \tilde{\mathbf{e}}^1 + (p_i/3 + \tilde{a}_2^\alpha) \tilde{\mathbf{e}}^2$ , similar to those in Appendix B.

Let  $\Delta V^{(p_i)}(\Phi_5^{(k)})$  be the contribution to the effective potential from  $\Phi_5^{(k)}$  with  $p_i$  defined in Eq. (5.2). Then, we obtain

$$\Delta V^{(p_i)}(\Phi_5^{(k)}) = 2 \sum_{\alpha=1}^5 \mathcal{V}^{(p_i)}(\tilde{a}_i^\alpha), \quad (5.14)$$

where the overall factor 2 on the right-hand side arises due to the real degrees of freedom of a complex scalar. The potential in Eq. (5.11) is manifestly invariant under integer shifts of an arbitrarily chosen component of the Wilson line phases,  $\tilde{a}_i^\alpha \rightarrow \tilde{a}_i^\alpha \pm 1$ , which preserve the Wilson line phase factors  $W_\ell$  in Eq. (3.29). Given the above invariance, we relax the traceless condition imposed in Eq. (5.7) as  $\sum_{\hat{a}=1}^5 \tilde{a}_{i+\hat{a}}^{\hat{a}} = 0 \pmod{1}$  in the following discussions.

We can generalize the above result to triplets belonging to other representations of  $SU(5)$ . Contributions to the effective potential depend on components of weight vectors with respect to the Cartan generators  $H_{\hat{a}}$ ; for a given representation  $\mathcal{R}$ , the representation matrix of  $H_{\hat{a}}$  is denoted by  $H_{\hat{a}}^{[\mathcal{R}]}$ . We can express eigenvalues of  $2\tilde{a}_{i+k}^{\hat{a}} H_{\hat{a}}^{[\mathcal{R}]}$  by using  $\tilde{a}_{i+k}^{\hat{a}}$ . Here, let us consider a threefold scalar  $\Phi_{\mathcal{R}}^{(k)}$ , which transforms under  $SU(5) \times SU(5) \times SU(5)$  as

$$\Phi_{\mathcal{R}}^{(1)} \sim (\mathcal{R}, \mathbf{1}, \mathbf{1}), \quad \Phi_{\mathcal{R}}^{(2)} \sim (\mathbf{1}, \mathcal{R}, \mathbf{1}), \quad \Phi_{\mathcal{R}}^{(3)} \sim (\mathbf{1}, \mathbf{1}, \mathcal{R}). \quad (5.15)$$

We write the contributions to the effective potential generated by  $\Phi_{\mathcal{R}}^{(k)}$  as  $\Delta V^{(p_i)}(\Phi_{\mathcal{R}}^{(k)})$ . We find that the contributions from, *e.g.*,  $\mathcal{R} = \mathbf{10}, \mathbf{15}, \mathbf{24}$  cases are given by

$$\Delta V^{(p_i)}(\Phi_{\mathbf{10}}^{(k)}) = 2 \sum_{1 \leq \alpha < \beta \leq 5} \mathcal{V}^{(p_i)}(\tilde{a}_i^\alpha + \tilde{a}_i^\beta), \quad (5.16)$$

$$\Delta V^{(p_i)}(\Phi_{\mathbf{15}}^{(k)}) = 2 \sum_{1 \leq \alpha \leq \beta \leq 5} \mathcal{V}^{(p_i)}(\tilde{a}_i^\alpha + \tilde{a}_i^\beta), \quad (5.17)$$

$$\Delta V^{(p_i)}(\Phi_{\mathbf{24}}^{(k)}) = 2 \sum_{1 \leq \alpha \neq \beta \leq 5} \mathcal{V}^{(p_i)}(\tilde{a}_i^\alpha - \tilde{a}_i^\beta), \quad (5.18)$$

respectively. Here, we have discarded irrelevant constants that are independent of  $\tilde{a}_i^\alpha$ .

For general threefold scalars in Eq. (4.3), we can derive a differential operator as in Eq. (5.9). As an example, let us consider an  $(\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3) = (\mathbf{5}, \mathbf{5}, \mathbf{1})$  case. In this case, a component of  $\Phi_{\mathcal{R}_{123}}^{(k)}$  has two indices, which we denote by  $\alpha_1$  and  $\alpha_2$  ( $\alpha_1, \alpha_2 = 1, \dots, 5$ ). Corresponding to Eq. (5.9), we find the following differential operator:

$$\hat{M}_{k, \alpha_1, \alpha_2}^2 = \frac{2}{3} \sum_{\ell=1}^3 \left( -i \partial_{y^\ell} + \frac{\tilde{a}_{k+\ell}^{\alpha_1} + \tilde{a}_{k+\ell+1}^{\alpha_2}}{R} \right)^2. \quad (5.19)$$

From the above, we obtain a one-loop correction to the potential from  $\Phi_{\mathcal{R}_{123}}^{(k)}$  in a similar way to the previous cases. The result is given by

$$\Delta V^{(p_i)}(\Phi_{\mathcal{R}_{123}}^{(k)}) = 2 \sum_{\alpha_1, \alpha_2=1}^5 \mathcal{V}^{(p_i)}(\tilde{a}_i^{\alpha_1} + \tilde{a}_{i+1}^{\alpha_2}). \quad (5.20)$$

We note that, except for the subscripts of the phases, the potential contribution coincides with the sum of those coming from  $\Phi_{\mathbf{10}}^{(k)}$  and  $\Phi_{\mathbf{15}}^{(k)}$ , which is an explicit example of the modification explained below Eq. (4.16).

We turn to discuss the contributions to the effective potential from threefold fermions. The contributions mostly depend on the eigenvalues of differential operators as in Eq. (5.9). Since the covariant derivatives for bosons and fermions are the same if they belong to the same representation of  $SU(5)$ , the eigenvalues are also common for bosons and fermions. Thus, the contributions from threefold fermions can be written by using the contributions from threefold boson. We denote a 6D Weyl fermion  $\Psi_{\mathcal{R}}^{\pm(k)}$ , whose representation is the same as in Eq. (5.15). A contribution to the effective potential from  $\Psi_{\mathcal{R}}^{\pm(k)}$  is denoted by  $\Delta V^{(p_i)}(\Psi_{\mathcal{R}}^{(k)})$ . Then, we find  $\Delta V^{(p_i)}(\Psi_{\mathcal{R}}^{(k)}) = -2\Delta V^{(p_i)}(\Phi_{\mathcal{R}}^{(k)})$ .

## B. Contributions from $\mathbb{Z}_3^{(\text{ex})}$ onefold fields

We start to discuss the contributions from  $\mathbb{Z}_3^{(\text{ex})}$  onefolds. We first examine a bulk matter scalar  $\Phi_{5^3}$ , whose component is written by  $(\Phi_{5^3})_{\alpha_1 \alpha_2 \alpha_3}$ . Here, the Greek indices run from 1 to 5. The BCs can be introduced as

$$(\Phi_{\mathbf{5}^3})_{\alpha_1\alpha_2\alpha_3}(x^\mu, \hat{T}_1[y^i]) = \omega^{p_t}(\Phi_{\mathbf{5}^3})_{\alpha_1\alpha_2\alpha_3}(x^\mu, y^i), \quad (5.21)$$

$$(\Phi_{\mathbf{5}^3})_{\alpha_1\alpha_2\alpha_3}(x^\mu, \hat{S}_0[y^i]) = \omega^{p_s}(\Phi_{\mathbf{5}^3})_{\alpha_3\alpha_1\alpha_2}(x^\mu, y^i). \quad (5.22)$$

The extradimensional component of the covariant derivative acting on  $(\Phi_{\mathbf{5}^3})_{\alpha_1\alpha_2\alpha_3}$  is written by

$$\langle D_{y^i} \rangle_{\alpha_1\alpha_2\alpha_3}^{\beta_1\beta_2\beta_3} = \delta_{\alpha_1}^{\beta_1} \delta_{\alpha_2}^{\beta_2} \delta_{\alpha_3}^{\beta_3} \left[ \partial_{y^i} + i \frac{2}{R} (\tilde{a}_{i+1}^{\alpha_1} + \tilde{a}_{i+2}^{\alpha_2} + \tilde{a}_{i+3}^{\alpha_3}) \right], \quad (5.23)$$

where the indices  $\alpha_k$  ( $k = 1, 2, 3$ ) are not summed on the right-hand side in the above.

As discussed in Sec. IV C,  $(\Phi_{\mathbf{5}^3})_{\alpha_1\alpha_2\alpha_3}$  contains  $Z_3^{\text{(ex)}}$  triplets and singlets. The latter corresponds to the components of  $\alpha_1 = \alpha_2 = \alpha_3$ . From Eq. (5.23), it is clear that the singlet does not couple to the Wilson line phases since  $\tilde{a}_{i+1}^{\alpha} + \tilde{a}_{i+2}^{\alpha} + \tilde{a}_{i+3}^{\alpha} = 0$  holds. Thus, only  $Z_3^{\text{(ex)}}$  triplets can give contribution to the effective potential.

For a set of fixed values of  $\{\alpha_1, \alpha_2, \alpha_3\}$ , a triplet is given by

$$\{(\Phi_{\mathcal{R}^3})_{\alpha_1\alpha_2\alpha_3}, (\Phi_{\mathcal{R}^3})_{\alpha_3\alpha_1\alpha_2}, (\Phi_{\mathcal{R}^3})_{\alpha_2\alpha_3\alpha_1}\} \equiv \{\phi^{(1)}, \phi^{(2)}, \phi^{(3)}\}. \quad (5.24)$$

One can see that  $\phi^{(k)}$  couples to the Wilson line phases of  $\tilde{a}_{i+k}^{\alpha_1} + \tilde{a}_{i+1+k}^{\alpha_2} + \tilde{a}_{i+2+k}^{\alpha_3}$  via the covariant derivative in Eq. (5.23). Then, as in Eq. (5.10), a KK mode of the triplet  $\phi^{(k)}$  has the following KK mass:

$$M_{k,\alpha_1,\alpha_2,\alpha_3}^2 = \frac{2}{3R^2} \sum_{\ell=1}^3 (N_\ell + \tilde{a}_{k+\ell}^{\alpha_1} + \tilde{a}_{k+\ell+1}^{\alpha_2} + \tilde{a}_{k+\ell+2}^{\alpha_3})^2. \quad (5.25)$$

This implies that a contribution to the effective potential from the triplet  $\phi^{(k)}$  is proportional to  $\mathcal{V}^{(p_t)}(\tilde{a}_i^{\alpha_1} + \tilde{a}_{i+1}^{\alpha_2} + \tilde{a}_{i+2}^{\alpha_3})$ .

Let  $\Delta V^{(p_t)}(\Phi_{\mathbf{5}^3})$  be the contribution from the onefold  $\Phi_{\mathbf{5}^3}$ . Among  $5^3 = 125$  components of  $(\Phi_{\mathbf{5}^3})_{\alpha_1\alpha_2\alpha_3}$ , five components are singlets, which give constants independent of the Wilson line phases. The remaining 120 components compose 40 triplets. We can take summations of the contributions from the triplets as

$$\Delta V^{(p_t)}(\Phi_{\mathbf{5}^3}) = \frac{2}{3} \left( \sum_{\alpha_1,\alpha_2,\alpha_3=1}^5 - \sum_{\alpha_1=\alpha_2=\alpha_3=1}^5 \right) \times \mathcal{V}^{(p_t)}(\tilde{a}_i^{\alpha_1} + \tilde{a}_{i+1}^{\alpha_2} + \tilde{a}_{i+2}^{\alpha_3}), \quad (5.26)$$

where on the right-hand side the overall factor appears since  $\Phi_{\mathbf{5}^3}$  is a complex scalar, and the factor  $1/3$  should be included to correctly count 40 triplets composed of 120 components. Let us note that the subtracted  $\alpha_1 = \alpha_2 = \alpha_3$

contributions in Eq. (5.26) are constant, which do not affect the vacuum structure of the potential.

Generalizations to the other representation than  $\mathbf{5}$  are straightforward. For example, we find that the contribution from  $\Phi_{\mathbf{10}^3}$  is given by

$$\Delta V^{(p_t)}(\Phi_{\mathbf{10}^3}) = \frac{2}{3} \left( \left[ \prod_{i=1}^3 \sum_{1 \leq \alpha_i < \beta_i \leq 5} \right] - \sum_{(\alpha_1,\beta_1)=(\alpha_2,\beta_2)=(\alpha_3,\beta_3)} \right) \times \mathcal{V}^{(p_t)}(\tilde{a}_i^{\alpha_1} + \tilde{a}_i^{\beta_1} + \tilde{a}_{i+1}^{\alpha_2} + \tilde{a}_{i+1}^{\beta_2} + \tilde{a}_{i+2}^{\alpha_3} + \tilde{a}_{i+2}^{\beta_3}), \quad (5.27)$$

where the above potential consists of the contributions from  $(10^3 - 10)/3 = 330$  triplets. As in the case of the threefold scalar, difference between contributions from the onefold scalars and fermions is just an overall factor. Let  $\Delta V^{(p_t)}(\Psi_{\mathcal{R}^3})$  be the contribution to the potential from a fermion  $\Psi_{\mathcal{R}^3}^\pm$ . Then, it follows that  $\Delta V^{(p_t)}(\Psi_{\mathcal{R}^3}) = -2\Delta V^{(p_t)}(\Phi_{\mathcal{R}^3})$ , where the contribution does not depend on 6D chiralities of fermions.

## VI. GAUGE SYMMETRY BREAKING PATTERNS IN $SU(5)$ MODELS

### A. Vacuum structure and unbroken gauge symmetries

We study the vacuum structure of the effective potential for the Wilson line phases derived in the previous section. For simplicity, we only consider the contributions to the potential from the gauge fields and threefold fields of  $\Phi_{\mathcal{R}}^{(k)}$  and  $\Psi_{\mathcal{R}}^{\pm(k)}$  for  $\mathcal{R} = \mathbf{5}, \mathbf{10}, \mathbf{15}, \mathbf{24}$ . First, for a chosen  $\mathcal{R}$ , we numerically find VEVs of the Wilson line phases at a global minimum of a contribution  $\Delta V^{(p_t)}(\Phi_{\mathcal{R}}^{(k)})$  or  $\Delta V^{(p_t)}(\Psi_{\mathcal{R}}^{(k)})$ . In the fundamental representation of  $SU(5)$ , the Wilson line phase factors  $W_\ell$  in Eq. (3.29) take the following form:

$$W_\ell = \text{diag}(e^{2\pi i \tilde{a}_{\ell+1}^1}, e^{2\pi i \tilde{a}_{\ell+1}^2}, e^{2\pi i \tilde{a}_{\ell+1}^3}, e^{2\pi i \tilde{a}_{\ell+1}^4}, e^{2\pi i \tilde{a}_{\ell+1}^5}) \otimes \text{diag}(e^{2\pi i \tilde{a}_{\ell+2}^1}, e^{2\pi i \tilde{a}_{\ell+2}^2}, e^{2\pi i \tilde{a}_{\ell+2}^3}, e^{2\pi i \tilde{a}_{\ell+2}^4}, e^{2\pi i \tilde{a}_{\ell+2}^5}) \otimes \text{diag}(e^{2\pi i \tilde{a}_\ell^1}, e^{2\pi i \tilde{a}_\ell^2}, e^{2\pi i \tilde{a}_\ell^3}, e^{2\pi i \tilde{a}_\ell^4}, e^{2\pi i \tilde{a}_\ell^5}). \quad (6.1)$$

Thus, if a VEV at a minimum is determined, we can find a gauge symmetry breaking pattern through Eqs. (3.27) and (6.1).

Before starting to show results, let us mention that there are degenerate vacua in potentials for the Wilson line phases. The degeneracy is related to the invariance of the potential under some transformations of the Wilson line phases. As we mentioned below Eq. (5.14),  $\mathcal{V}^{(p_t)}(\tilde{a}_i^\alpha)$  in Eq. (5.11) is invariant under an integer shift  $\tilde{a}_i^\alpha \rightarrow \tilde{a}_i^\alpha \pm 1$ . Thus, effective potentials for the Wilson line phases generally have degeneracy related to the integer shift invariance. This is due to the phase property of  $\tilde{a}_i^\alpha$ . In addition, from Eq. (5.11), we see that a simultaneous



TABLE I. The values of  $\tilde{a}_i^\alpha$  at a global minimum of the contributions  $\Delta V^{(p_i)}(\phi)$ , where  $\phi$  is  $\Phi_{\mathcal{R}}^{(k)}$  or  $\Psi_{\mathcal{R}}^{\pm(k)}$  for  $\mathcal{R} = 5, 10, 15, 24$ . We also show the unbroken gauge symmetry  $G_0$  at the minimum. The constant  $v_x = 0.24796$  is used.

$\mathcal{R}$	Potential	$(\tilde{a}_1^1, \tilde{a}_1^2, \tilde{a}_1^3, \tilde{a}_1^4, \tilde{a}_1^5)$	$(\tilde{a}_2^1, \tilde{a}_2^2, \tilde{a}_2^3, \tilde{a}_2^4, \tilde{a}_2^5)$	$G_0$
<b>5</b>	$\Delta V^{(0)}(\Phi_5^{(k)})$	(0, 0, 0, 0, 0)	(0, 0, 0, 0, 0)	$SU(5)$
	$\Delta V^{(1)}(\Phi_5^{(k)})$	(3, 3, 3, 3, 3)/5	(3, 3, 3, 3, 3)/5	$SU(5)$
	$\Delta V^{(0)}(\Psi_5^{(k)})$	(2, 1, 1, 1, 1)/3	(2, 1, 1, 1, 1)/3	$SU(4) \times U(1)$
	$\Delta V^{(1)}(\Psi_5^{(k)})$	(0, 0, 0, 0, 0)	(0, 0, 0, 0, 0)	$SU(5)$
<b>10</b>	$\Delta V^{(0)}(\Phi_{10}^{(k)})$	(0, 0, 0, 0, 0)	(0, 0, 0, 0, 0)	$SU(5)$
	$\Delta V^{(1)}(\Phi_{10}^{(k)})$	(2, 2, 2, 2, 2)/5	(4, 4, 4, 4, 4)/5	$SU(5)$
	$\Delta V^{(0)}(\Psi_{10}^{(k)})$	(1, 1, 1, 1, 1)/5	(1, 1, 1, 1, 1)/5	$SU(5)$
	$\Delta V^{(1)}(\Psi_{10}^{(k)})$	(0, 0, 0, 0, 0)	(0, 0, 0, 0, 0)	$SU(5)$
<b>15</b>	$\Delta V^{(0)}(\Phi_{15}^{(k)})$	(0, 0, 0, 0, 0)	(0, 0, 0, 0, 0)	$SU(5)$
	$\Delta V^{(1)}(\Phi_{15}^{(k)})$	(2, 2, 2, 2, 2)/5	(4, 4, 4, 4, 4)/5	$SU(5)$
	$\Delta V^{(0)}(\Psi_{15}^{(k)})$	(2, 1, 1, 1, 1)/6	(2, 1, 1, 1, 1)/6	$SU(4) \times U(1)$
	$\Delta V^{(1)}(\Psi_{15}^{(k)})$	(0, 0, 0, 0, 0)	(0, 0, 0, 0, 0)	$SU(5)$
<b>24</b>	$\Delta V^{(0)}(\Phi_{24}^{(k)})$	(0, 0, 0, 0, 0)	(0, 0, 0, 0, 0)	$SU(5)$
	$\Delta V^{(1)}(\Phi_{24}^{(k)})$	(1, 1, 2, 2, 0)/3	(1, 1, 2, 2, 0)/3	$SU(2)^2 \times U(1)^2$
	$\Delta V^{(0)}(\Psi_{24}^{(k)})$	(1/3, 2/3, 0, $v_x$ , $1 - v_x$ )	(1/3, 2/3, $v_x$ , $1 - v_x$ , 0)	$U(1)^4$
	$\Delta V^{(1)}(\Psi_{24}^{(k)})$	(0,0,0,0,0)	(0,0,0,0,0)	$SU(5)$

change of the overall sign of the VEVs as  $\tilde{a}_i^\alpha \rightarrow -\tilde{a}_i^\alpha$  for  $i = 1, 2$  and  $\alpha = 1-5$  does not change the potentials for  $p_i = 0$  cases. This leads to a degeneracy in the potentials. On the other hand, the contributions to the potentials from fields with  $p_i = 1$  and  $-1$  are related to each other by the overall sign change of the phases, i.e.,  $\mathcal{V}^{(-1)}(\tilde{a}_i^\alpha) = \mathcal{V}^{(1)}(-\tilde{a}_i^\alpha)$ , which is shown from Eq. (5.11). The potentials are invariant under the permutation of the index  $\alpha$ , which can be regarded as a basis change in the representation space. The exchange of  $\tilde{a}_1^\alpha$  and  $\tilde{a}_2^\alpha$  also does not change the potentials. Finally, the potential contributions from adjoint matter fields are invariant under the  $\mathbb{Z}_5$  transformation, which is the center subgroup of  $SU(5)$ , with  $\tilde{a}_i^\alpha + n_i/5$  ( $i = 1, 2$ ), where  $n_i \in \mathbb{Z}$ .

Concerning the above degeneracy, in the following, we show representatives of VEVs at a degenerate global minimum. In Table I, we show the values of  $\tilde{a}_i^\alpha$  at a global minimum of each contribution of  $\Delta V^{(p_i)}(\Phi_{\mathcal{R}}^{(k)})$  and  $\Delta V^{(p_i)}(\Psi_{\mathcal{R}}^{(k)})$  for  $p_i = 0, 1$  and  $\mathcal{R} = 5, 10, 15, 24$ . As noted below Eq. (5.14), the traceless condition holds modulo 1. We also show the unbroken gauge symmetry  $G_0$  at the minimum. We don't give explicit results of

$p_i = -1$  cases since they are obtained from the ones of  $p_i = 1$  cases through the relation  $\mathcal{V}^{(-1)}(\tilde{a}_i^\alpha) = \mathcal{V}^{(1)}(-\tilde{a}_i^\alpha)$  explained above.

The gauge field also generates the contribution to the effective potential, which is equal to  $2\Delta V^{(0)}(\Phi_{24}^{(k)})$ , whose minimum respects  $SU(5)$  symmetry. Thus, we need bulk matter fields in the theory to obtain the SM gauge symmetry  $G_{\text{SM}} \equiv SU(3) \times SU(2) \times U(1)$  at a vacuum. Let us remark that  $2\Delta V^{(0)}(\Phi_{24}^{(k)}) + \Delta V^{(0)}(\Psi_{24}^{(k)}) = 0$  at the one-loop level, and the contribution  $\Delta V^{(1)}(\Psi_5^{(k)})$  has degenerate global minima with  $G_{\text{SM}}$  and  $SU(5)$ , as seen in Table I. Thus, we easily find matter contents that ensure  $G_{\text{SM}}$  at a minimum and have no bulk and boundary anomalies. We show two examples in Table II. We refer to the bulk matter contents shown in the left and right tables as case (i) and (ii), respectively. The case (i) consists of a  $p_i = 0$  adjoint threefold fermion with positive chirality and 10 sets of the  $p_i = 1$  fundamental threefold fermion with negative chirality. The case (ii) consists of a  $p_i = 0$  adjoint threefold fermion with positive chirality, the 16 sets of the  $p_i = 1$  fundamental threefold fermion with negative chirality, and the two sets of the  $p_i = 0$  antisymmetric

TABLE II. Examples of bulk matter contents. We refer to the matter contents of the left (right) table as the case (i) (case (ii)).

Case (i)		
Bulk matter	$p_t$	Flavor
$\Psi_{24}^{+(k)}$	0	1
$\Psi_5^{-(k)}$	1	10
Case (ii)		
Bulk matter	$p_t$	Flavor
$\Psi_{24}^{+(k)}$	0	1
$\Psi_5^{-(k)}$	1	16
$\Psi_{10}^{-(k)}$	0	2

(10-dimensional) representation threefold fermion with negative chirality.<sup>7</sup> In both cases, one sees that there are no anomalies. In addition, the potential contributions from the gauge field and an adjoint fermion field cancel out. For the case (i), the sum of the effective potential contributions is proportional to  $\Delta V^{(1)}(\Psi_5^{(k)})$ , in which  $SU(5)$  and  $G_{SM}$  vacua are degenerate. For the case (ii), we numerically find that, at the global minima of the effective potential, the values of the Wilson line take

$$\tilde{a}_1^\alpha = \tilde{a}_2^\alpha = (1, 1, 1, 0, 0)/3, \quad (6.2)$$

and the symmetry  $SU(5)$  is broken down to  $G_{SM}$ . We note that on this vacuum  $\tilde{a}_3^\alpha = (-2, -2, -2, 0, 0)/3$  and  $\tilde{a}_\ell^\alpha - \tilde{a}_{\ell+1}^\alpha = 0 \pmod{1}$  are obtained. Thus, this vacuum respects the symmetry  $\mathbb{Z}_3^{(+)} \times \mathbb{Z}_3^{(-)} \cong \mathbb{Z}_3^{(ex)} \times \mathbb{Z}_3^{(L)}$ , as discussed in Sec. III C.

## B. Phenomenological implications

On the vacuum shown in Eq. (6.2), interestingly, the so-called doublet-triplet splitting among the Higgs fields in the **5** representation can be realized, similarly in the  $S^1/\mathbb{Z}_2$  case [16].

If we introduce a **5** threefold scalar with  $p_t = 0$ , its triplet component gets contribution from the Wilson line phases to become massive, while its doublet component does not and contains a massless mode. We note that on this vacuum, the  $\mathbb{Z}_3^{(ex)}$  symmetry remains unbroken, even though the zero modes of the extradimensional components of the gauge fields which develop nonvanishing VEV,  $A_{y^i}$ , have non-trivial charges of the  $\mathbb{Z}_3^{(ex)}$  symmetry. This means that the tadpole term of the zero mode of  $A_{y^i}$  is absent even in the higher-loop corrections to allow the vacuum to be a (local)

<sup>7</sup>The same  $SU(5)$  representations of the fermionic sector are found in one of the supersymmetric models in [30].

minimum without a fine tuning. In addition, the effective theory around the TeV scale would have a  $\mathbb{Z}_3$  symmetry, though a soft-breaking term of the  $\mathbb{Z}_3$  symmetry may be introduced as in the  $S^1/\mathbb{Z}_2$  case [17].

Of course, there would be large radiative corrections to the scalar masses in nonsupersymmetric (non-SUSY) models, and thus we impose the SUSY in following. In the SUSY limit, however, the contributions from the fermions and the bosons to the effective potential are canceled out. Thus, the actual effective potential strongly depends on the SUSY breaking. In addition, when there is a hierarchy between the SUSY-breaking scale and the compactification scale, the effective potential suffers from the large logarithms, and we need to treat the renormalization group equations. In this way, the analysis in the previous subsection can not be applied directly. Nevertheless, it provides a hope that the vacuum tends to be realized in a sizable parameter region, besides a proof of existence.

Concerning the vacuum selection, we have proposed an interesting scenario in Ref. [18], which may be applied also to the present case. In the reference, we have calculated the effective potential at a finite temperature and found that there are models where the desired vacuum (in the  $S^1/\mathbb{Z}_2$  case) is the global minimum at high temperature. Thus, if the universe started with very high temperature of order the Planck scale, the vacuum would be selected around the temperature of order the compactification/GUT scale, before the inflation. Then, it is natural to expect that the vacuum does not move so much until the reheating and has been selected.

An outstanding prediction of the SUSY version is the existence of light adjoint chiral supermultiplets of masses around the SUSY-breaking scale, which would be a TeV scale. This is understood as follows. The zero modes of  $A_{y^i}$  are massless at the tree level and receive masses through radiative corrections that are suppressed by the SUSY-breaking scale. Since the mass differences among components in a single supermultiplet are at most of the SUSY-breaking scale, the masses of their SUSY partners are also at most of the scale. Some collider phenomenology of them in the  $S^1/\mathbb{Z}_2$  case was studied in Ref. [17]. In Ref. [19], another attractive possibility to regard the adjoint chiral supermultiplets as those introduced in the Dirac gaugino scenario [31] is studied to show that the so-called goldstone gauginos [32] are naturally realized. Similar analyses in the present case are desirable.

An unfavorable point of this prediction is that the light adjoint chiral supermultiplets ruin the success of the gauge coupling unification in the minimal SUSY  $SU(5)$  model [3]. This is because the adjoint multiplets give contributions of  $\Delta b_i^{adj} = (0, 2, 3)$  for the beta function coefficients to that of the minimal supersymmetric SM (MSSM),  $b_i^{MSSM} = (33/5, 1, -3)$ . It is possible, however, to recover the gauge coupling unification, for example by

introducing additional multiplets that give further correction of  $\Delta b_i^{add} = (3 + n, 1 + n, n)$  [16].

It is notable that an example with  $n = 0$  is naturally realized in the present case, for instance by adding one **5** and two **10** threefold hypermultiplets with  $p_i = 0$ . This is because the above **5** (**10**) hypermultiplet contains a zero mode vectorlike pairs of the component with the SM charge  $(\mathbf{1}, \mathbf{2})_{-1/2}$  ( $(\mathbf{1}, \mathbf{1})_1$ ). We note that it is in contrast to the  $S^1/\mathbb{Z}_2$  case, where the pair with  $(\mathbf{1}, \mathbf{1})_1$  can not be realized separately. This difference would bring significant effects on the phenomenology as the quantum corrections to the colored particles are not so enhanced in contrast to the  $n = 1$  case where the color  $SU(3)$  symmetry is asymptotic nonfree (though still perturbative around the GUT scale) [17].

Next, we discuss the matter sector. As shown in Sec. IV C, the zero modes of the threefold fermions are vector-like, and those of the onefold fermions may be chiral but the possible representations are restricted. Then, the simplest way to realize the chiral fermion in the SM is to put them on the fixed points. Though there are still several possibilities to put the fermions on the three fixed points, we consider here only the case all the SM fermions are put on a common fixed point, for simplicity.

In contrast to the usual gauge-Higgs unification models where the SM Higgs field is unified into a gauge field, the SM Higgs field is introduced as a **5** field in our scenario, and its Yukawa coupling can be set by hand on the fixed point. The flavor structure of the Yukawa couplings is similar to usual 4D models and it might be set by hand or a flavor symmetry may be introduced. A difference from the usual 4D models is the  $SU(5)$  breaking effect, which is carried only by  $A_{y_i}$ , and thus bulk fermions are necessary as messenger of the  $SU(5)$  breaking, to solve the wrong GUT relation among the Yukawa couplings.

Finally, we comment on the  $\mu$  problem and the proton decay. If we put a **5** threefold hypermultiplet with negative chirality and  $p_i = 0$ , the zero modes are a vectorlike pair of the doublet chiral supermultiplet with the  $\mathbb{Z}_3$ -charge  $+1$ . When these are identified with  $H_u$  and  $H_d$  of the MSSM, the matter chiral supermultiplet  $\mathbf{10}_i$  and  $\bar{\mathbf{5}}_i$  where the index  $i$  denotes the generation should have the  $\mathbb{Z}_3$  charge  $+1$  to allow the Yukawa couplings. These  $\mathbb{Z}_3$  charge forbids the dimension 5 operator for the proton decay,  $\mathbf{10}_i \mathbf{10}_j \mathbf{10}_k \bar{\mathbf{5}}_l$ , and, at the same time, the  $\mu$  term in the MSSM. We suppose the SUSY breaking sector breaks the  $\mathbb{Z}_3$  symmetry softly to solve the  $\mu$  problem. Though this  $\mathbb{Z}_3$  breaking may generate the dimension-5 proton decay operator, its contribution to the proton decay is quite suppressed. Then, the proton decay via the dimension-6 operators mediated by the gauge field becomes dominant. In the 6D spacetime, the sum of the contributions from the KK gauge boson is (logarithmically) divergent [33], when all the fermion fields are put on a single fixed point. Though the summation should be cut off at some point as the 6D theory is also an effective

theory, this process is enhanced, besides the effect of the enhanced coupling of the KK gauge field and the boundary fermions by a factor  $\sqrt{3}$  shown in Eq. (3.17). Meanwhile, it also has a suppression factor. It is possible that the dominant element of the SM fermion may come from the ‘‘messenger field’’ instead of the boundary fields. In case that the origins of the dominant modes of the components of each  $SU(5)$  multiplet are different, the gauge interactions do not connect them. These points should be studied in a future work.

## VII. CONCLUSIONS AND DISCUSSIONS

We have formulated a field theoretical realization of the diagonal embedding method in the gauge theory compactified on the  $T^2/\mathbb{Z}_3$  orbifold. The original bulk gauge group of the theory is  $G \times G \times G$ , and a global  $\mathbb{Z}_3^{(ex)}$  transformation permutes them. Through the BCs, only the diagonal part of the gauge group  $G^{diag}$ , which is isomorphic to  $G$ , remains manifest at a low-energy effective theory. The 4D effective theory contains the zero mode of the extra-dimensional component of the gauge field, which belongs to the adjoint representation of  $G^{diag}$ . The continuous Wilson line phase degrees of freedom, i.e., the zero mode along the flat direction of the tree-level potential for the extradimensional gauge fields, can acquire VEVs that further spontaneously break the gauge symmetry  $G^{diag}$ . Thus, the theory possesses rich vacuum structure. We have shown a parametrization of the VEVs and the Wilson line phases, which are required to clarify the symmetry breaking patterns.

We have also discussed the bulk scalar and fermion fields in our setup. The representations of these bulk matter fields under the gauge group are restricted to be the  $\mathbb{Z}_3^{(ex)}$  threefold or onefold to keep the  $\mathbb{Z}_3^{(ex)}$  invariance of the Lagrangian. We have examined the possible BCs for the matter fields and the KK mass spectrum. The onefold fermions can have 4D chiral fermions as their zero modes, although the threefold ones always have vectorlike 4D fermion zero modes. A particular feature is that the representations of the chiral zero modes under the gauge group are restricted due to the diagonal embedding method, as shown in Eqs. (4.49) and (4.50).

We have studied the  $SU(5)$  type A grand gauge-Higgs unification model compactified on  $T^2/\mathbb{Z}_3$  with the diagonal embedding method as an explicit application. We have derived the one-loop contributions to the effective potential for the zero modes of extradimensional gauge fields. We have examined the vacuum structure of the effective potential and discussed the symmetry breaking patterns related to the bulk matter contents. Our analysis has shown that the  $SU(5)$  symmetry is broken down to  $SU(3) \times SU(2) \times U(1)$  at the global minima of the effective potential with the specific bulk matter contents. Thus,

the type A grand gauge-Higgs unification model on  $T^2/\mathbb{Z}_3$  is viable for explaining the spontaneous GUT breaking.

In the present analysis, we utilize the dual-lattice technique, which is just a Fourier transformation. It is actually useful to analyze the KK expansion in the  $T^2/\mathbb{Z}_3$  model, which is the minimal  $\mathbb{Z}_3$  orbifold model and may be regarded as an effective theory of the heterotic string theory with an adjoint scalar zero mode and with three generations. In addition, this technique can be applied to more general orbifold models, for instance in a ten-dimensional spacetime, straightforwardly. It is also possible to treat more general gauge symmetry than  $SU(5)$  considered in this article, such as  $SO(10)$ ,  $E_6$  and  $E_8$ . These generalizations would be attractive future works.

Finally, we have discussed the phenomenological implications qualitatively, focusing on the GUT breaking vacuum. A notable feature of this spontaneous GUT breaking is to provide a solution to the doublet-triplet splitting problem in GUT models. In addition, the vacuum is characterized by the enhancement of a  $\mathbb{Z}_3$  symmetry and is implied to be stable against higher-loop quantum corrections. With a SUSY extension, the light three chiral supermultiplets, which are adjoint representations under  $SU(3)$ ,  $SU(2)$ , or  $U(1)$ , are predicted to appear around the SUSY-breaking scale. The unification of the three gauge couplings in the SM can be consistently explained with the vanishing beta function coefficient of the color  $SU(3)$  at the one-loop order. We have also given discussions about the SM matter sector and proton decay, although detailed examinations are left for future studies.

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## APPENDIX A: KALZUA-KLEIN EXPANSIONS ON $M^4 \times T^2/\mathbb{Z}_3$

In this appendix, we discuss the KK expansion on  $M^4 \times T^2/\mathbb{Z}_3$ . In the following, we regard  $\hat{T}_1$  and  $\hat{S}_0$  as the independent operators among  $\hat{T}_{1,2}$  and  $\hat{S}_{0,1,2}$  defined in Sec. II.

### 1. $\mathbb{Z}_3^{(\text{ex})}$ singlet fields

We first discuss the KK expansion of  $\mathbb{Z}_3^{(\text{ex})}$  singlet fields. Let  $\phi(x^\mu, y^i)$  be a  $\mathbb{Z}_3^{(\text{ex})}$  singlet field that obeys the BCs as

$$\begin{aligned}\phi(x^\mu, \hat{T}_1[y^i]) &= \omega^{p_t} \phi(x^\mu, y^i), \\ \phi(x^\mu, \hat{S}_0[y^i]) &= \omega^{p_s} \phi(x^\mu, y^i),\end{aligned}\quad (\text{A1})$$

where  $p_t, p_s \in \{0, \pm 1\}$ , which are consistent with  $\hat{S}_r^3 = \hat{T}_r$  ( $r = 0, 1, 2$ ).

To examine the KK expansion, we introduce the orthonormalized eigenfunction under the translation  $\bar{y}^i \rightarrow \hat{T}_j[\bar{y}^i] = \bar{y}^i + \delta_j^i$  ( $i, j = 1, 2$ ), where  $\bar{y}^i = y^i/(2\pi R)$ , as

$$f(\bar{y}^i(n_i + \alpha_i)) = \frac{1}{2\pi R(\det g_{ij})^{1/4}} e^{2\pi i \bar{y}^i(n_i + \alpha_i)},$$

$$n_i \in \mathbb{Z}, \quad \alpha_i \in \mathbb{R}. \quad (\text{A2})$$

One sees the eigenfunction satisfies

$$f(\hat{T}_j[\bar{y}^i](n_i + \alpha_i)) = e^{2\pi i \alpha_j} f(\bar{y}^i(n_i + \alpha_i)), \quad (\text{A3})$$

$$\iint_{T^2} d^2 y f^*(\bar{y}^i(n_i + \alpha_i)) f(\bar{y}^j(n'_j + \alpha_j)) = \delta_{n_1 n'_1} \delta_{n_2 n'_2} \equiv \delta_{n_i n'_i}^{(2)}, \quad (\text{A4})$$

where we have defined

$$\begin{aligned}\iint_{T^2} d^2 y &\equiv \int_0^{2\pi R} dy^1 \int_0^{2\pi R} dy^2 \sqrt{\det g_{ij}} \\ &= \frac{3}{4} \int_0^{2\pi R} dy^1 \int_0^{2\pi R} dy^2.\end{aligned}\quad (\text{A5})$$

As explained in Sec. II, a pair of the same upper and lower indices, such as  $i$  in Eq. (A3), is always contracted as  $\bar{y}^i n_i = \bar{y}^1 n_1 + \bar{y}^2 n_2$ .

Notice that  $f(\bar{y}^i(n_i + \alpha_i))$  is not an eigenfunction of the  $\mathbb{Z}_3$  transformation generated by  $\hat{S}_0$  defined in Eq. (2.9). Using Eq. (2.21), we see that the transformation of the function is

$$\begin{aligned}f(\hat{S}_0[\bar{y}^i](n_i + \alpha_i)) &= f(\bar{y}^i \hat{S}_0^{-1}[n_i + \alpha_i]) \\ &= f(\bar{y}^i(n_{i+1} + \alpha_{i+1})),\end{aligned}\quad (\text{A6})$$

where we have defined  $n_3 = -n_1 - n_2$ ,  $\alpha_3 = -\alpha_1 - \alpha_2$ ,  $n_{i+3} = n_i$ , and  $\alpha_{i+3} = \alpha_i$  for  $i \in \mathbb{Z}$ . The eigenfunction of both the transformations  $\hat{T}_1$  and  $\hat{S}_0$  is given by

$$\tilde{f}^{[p]}(\bar{y}^i N_i) = \frac{1}{\sqrt{3}} \sum_{k=1}^3 \omega^{-kp} f(\bar{y}^i N_{i+k}), \quad p \in \mathbb{Z}, \quad (\text{A7})$$

where

$$\begin{aligned}N_1 &\equiv n_1 + \frac{p_t}{3}, & N_2 &\equiv n_2 + \frac{p_t}{3}, \\ N_3 &\equiv -n_1 - n_2 - \frac{2p_t}{3}, & N_{i+3} &\equiv N_i.\end{aligned}\quad (\text{A8})$$

Conversely, we also obtain the relation as

$$f(\bar{y}^i N_{i+k}) = \frac{1}{\sqrt{3}} \sum_{p=-1}^1 \omega^{kp} \tilde{f}^{[p]}(\bar{y}^i N_i). \quad (\text{A9})$$

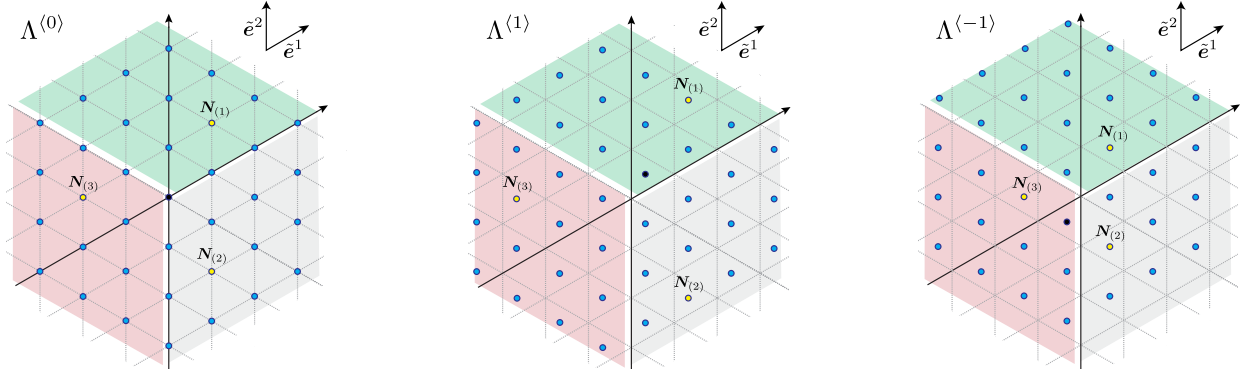


FIG. 2. The dual lattice  $\Lambda^{(p_t)}$  defined in Eq. (A12) for  $p_t = 0, 1, -1$ . The black dots show the point with  $n_1 = n_2 = 0$ . As an example, we denote  $N_{(\ell)}$  for  $n_1 = n_2 = 1$  by the yellow dots. Dots on the green, gray, and red-shaded regions belong to the sublattice  $\Lambda_{(1)}^{(p_t)}$ ,  $\Lambda_{(2)}^{(p_t)}$ , and  $\Lambda_{(3)}^{(p_t)}$  defined in Eq. (A14), respectively.

From Eq. (A7), one confirms

$$\begin{aligned}\tilde{f}^{[p_s]}(\mathcal{T}_j[\bar{y}^i]N_i) &= \omega^{p_t} \tilde{f}^{[p_s]}(\bar{y}^i N_i), \\ \tilde{f}^{[p_s]}(\mathcal{S}_0[\bar{y}^i]N_i) &= \omega^{p_s} \tilde{f}^{[p_s]}(\bar{y}^i N_i),\end{aligned}\quad (\text{A10})$$

where the eigenvalues are exactly the same as in Eq. (A1). Thus, a  $\mathbb{Z}_3^{(\text{ex})}$  singlet field with the BCs in Eq. (A1) is expanded by  $\tilde{f}^{[p_s]}(\bar{y}^i N_i)$ .<sup>8</sup>

The eigenfunctions in the set  $\{\tilde{f}^{[p]}(\bar{y}^i N_i)\}$  for  $n_i \in \mathbb{Z}$  are neither completely independent nor orthonormalized.<sup>9</sup> From the right of Eq. (A10) and Eq. (2.21), we find

$$\tilde{f}^{[p]}(\mathcal{S}_0^\ell[\bar{y}^i]N_i) = \tilde{f}^{[p]}(\bar{y}^i N_{i+\ell}) = \omega^{\ell p} \tilde{f}^{[p]}(\bar{y}^i N_i), \quad (\text{A11})$$

which implies a linear dependency  $\tilde{f}^{[p]}(\bar{y}^i N_{i+\ell}) \propto \tilde{f}^{[p]}(\bar{y}^i N_i)$  related to the  $\mathbb{Z}_3$  transformation. As seen below, there is no additional linear dependencies except for the above. To handle the eigenfunctions, it is convenient to introduce the normalized momentum lattice, which corresponds to the possible momentum values on  $T^2$  in a normalization and is expanded by the dual basis vector in Eq. (2.15) as

$$\begin{aligned}\Lambda^{(p_t)} &= \left\{ N_1 \tilde{e}^1 + N_2 \tilde{e}^2 = \left( n_1 + \frac{p_t}{3} \right) \tilde{e}^1 \right. \\ &\quad \left. + \left( n_2 + \frac{p_t}{3} \right) \tilde{e}^2 \mid n_1, n_2 \in \mathbb{Z} \right\}.\end{aligned}\quad (\text{A12})$$

<sup>8</sup>The eigenfunctions  $\tilde{f}^{[p_s]}(\bar{y}^i N_i)$  given by linear combinations of the exponential functions in Eq. (A2) are analogues to  $\sin(yn/R)$  or  $\cos(yn/R)$  ( $n \in \mathbb{Z}$ ) in  $S^1/\mathbb{Z}_2$  orbifold models.

<sup>9</sup>This is similar to the fact that  $\sin(yn/R)$  and  $\sin(-yn/R)$  is not linearly independent even if  $n \neq -n$  is satisfied. If one considers  $m, m' \in \mathbb{Z}_{>0}$ ,  $\sin(ym/R)$  and  $\sin(ym'/R)$  are linearly independent for  $m \neq m'$ .

We hereafter refer to  $\Lambda^{(p_t)}$  as the dual lattice. In Fig. 2, the dual lattice with  $p_t = 0, \pm 1$  is illustrated. Since we can relate  $N_{(\ell)}$  and  $N_{(\ell+1)}$  appearing in  $\tilde{f}^{[p]}(\bar{y}^i N_{i+\ell-1})$  to a point  $N_{(\ell)} \equiv N_{\ell} \tilde{e}^1 + N_{\ell+1} \tilde{e}^2$  on  $\Lambda^{(p_t)}$ , we regard that there is a corresponding eigenfunction on each point on the lattice. Note that  $N_{(1)}$ ,  $N_{(2)}$ , and  $N_{(3)}$  are not identical points on  $\Lambda^{(p_t)}$ , except for the case of  $(N_1, N_2) = (0, 0)$ . These points are related to each other by the  $\mathbb{Z}_3$  transformation generated by  $\hat{\mathcal{S}}_0$  as found in Eq. (A6) and identified to the positions of vertices of the equilateral triangle, whose center is located at the origin. From the above observation, we can divide  $\Lambda^{(p_t)}$  into the sublattice as<sup>10</sup>

$$\Lambda^{(p_t)} = \Lambda_{(1)}^{(p_t)} + \Lambda_{(2)}^{(p_t)} + \Lambda_{(3)}^{(p_t)} + \Lambda_{(0)} \delta_{p_t, 0}, \quad (\text{A13})$$

where

$$\begin{aligned}\Lambda_{(\ell)}^{(p_t)} &= \left\{ N_{(\ell)} = N_{\ell} \tilde{e}^1 + N_{\ell+1} \tilde{e}^2 \mid N_i = n_i + \frac{p_t}{3}, \right. \\ &\quad \left. n_1, n_2 \in \mathbb{Z}, N_2 \geq 0, N_1 > -N_2 \right\},\end{aligned}\quad (\text{A14})$$

for  $\ell = 1, 2, 3$  and  $\Lambda_{(0)}$  is the origin. If  $\tilde{f}^{[p]}(\bar{y}^i N_i)$  corresponds to a point on  $\Lambda_{(\ell)}^{(p_t)}$ , then the dependent function  $\tilde{f}^{[p]}(\bar{y}^i N_{i+1})$  corresponds to a point on  $\Lambda_{(\ell+1)}^{(p_t)}$ . Thus, we see that the set of the eigenfunctions  $\{\tilde{f}^{[p]}(\bar{y}^i N_i)\}$  defined on a sublattice  $\Lambda_{(\ell)}^{(p_t)}$  are linearly independent.

In the following, we use

$$N = N_1 \tilde{e}^1 + N_2 \tilde{e}^2 = \left( n_1 + \frac{p_t}{3} \right) \tilde{e}^1 + \left( n_2 + \frac{p_t}{3} \right) \tilde{e}^2, \quad (\text{A15})$$

<sup>10</sup>The decomposition in Eq. (A13) with  $p_t = 0$  corresponds to  $\mathbb{Z} = \mathbb{Z}_{>0} + \mathbb{Z}_{<0} + \{0\}$  in  $S^1/\mathbb{Z}_2$  orbifold models.

$$N' = N'_1 \tilde{e}^1 + N'_2 \tilde{e}^2 = \left(n'_1 + \frac{p_t}{3}\right) \tilde{e}^1 + \left(n'_2 + \frac{p_t}{3}\right) \tilde{e}^2. \quad (\text{A16})$$

With the help of  $\delta_{n_i+k, n'_{i+k'}}^{(2)} = \delta_{kk'} \delta_{n_i n'_i}^{(2)}$ , one can derive the orthonormal relation

$$\iint_{T^2} d^2 y \tilde{f}^{[p]*}(\bar{y}^i N_i) \tilde{f}^{[p']}(\bar{y}^i N'_i) = \delta_{n_i n'_i}^{(2)} \delta_{pp'}, \quad \text{for } N, N' \in \Lambda_{(\ell)}^{(p_t)}, \quad (\text{A17})$$

for a fixed  $\ell$ , from the definition of  $\tilde{f}^{[p]}(\bar{y}^i N_i)$  in Eq. (A7) and the relation in Eq. (A4).

Using the eigenfunction in Eq. (A7), we define the KK expansion of the singlet field in Eq. (A1) as follows:

$$\begin{aligned} \phi(x^\mu, y^i) &= \sum_{N \in \Lambda_{(\ell)}^{(p_t)}} \tilde{\phi}_{N_1, N_2}(x^\mu) \tilde{f}^{[p_s]}(\bar{y}^i N_i) \\ &+ \frac{\delta_{p_t, 0} \delta_{p_s, 0}}{2\pi R (\det g_{ij})^{1/4}} \tilde{\phi}_{0,0}(x^\mu), \end{aligned} \quad (\text{A18})$$

where we refer to  $\tilde{\phi}_{N_1, N_2}(x^\mu)$  as the KK mode. The zero mode in the last term exists only for the case with  $(p_t, p_s) = (0, 0)$ . We define the first term in Eq. (A18) to be independent of a choice of  $\ell$  in  $\Lambda_{(\ell)}^{(p_t)}$ . Thus, we can substitute  $\Lambda_{(\ell \mp 1)}^{(p_t)}$  for  $\Lambda_{(\ell)}^{(p_t)}$  in Eq. (A18) and use Eq. (A11) to get

$$\begin{aligned} &\sum_{N \in \Lambda_{(\ell)}^{(p_t)}} \tilde{\phi}_{N_1, N_2}(x^\mu) \tilde{f}^{[p_s]}(\bar{y}^i N_i) \\ &= \sum_{N \in \Lambda_{(\ell \mp 1)}^{(p_t)}} \tilde{\phi}_{N_1, N_2}(x^\mu) \omega^{\mp p_s} \tilde{f}^{[p_s]}(\bar{y}^i N_{i \pm 1}) \end{aligned} \quad (\text{A19})$$

$$= \sum_{N \in \Lambda_{(\ell)}^{(p_t)}} \omega^{\mp p_s} \tilde{\phi}_{N_{1 \mp 1}, N_{2 \mp 1}}(x^\mu) \tilde{f}^{[p_s]}(\bar{y}^i N_i). \quad (\text{A20})$$

This implies the constraint on the KK mode  $\tilde{\phi}_{N_1, N_2}(x^\mu)$  as

$$\tilde{\phi}_{N_{1 \pm \ell}, N_{2 \pm \ell}}(x^\mu) = \omega^{\mp \ell p_s} \tilde{\phi}_{N_1, N_2}(x^\mu). \quad (\text{A21})$$

Let us derive the effective 4D Lagrangian for the singlet field in Eq. (A1) from the KK expansion (A18). As an example, we treat  $\phi(x^\mu, y^i)$  as a scalar and consider the 6D canonical kinetic term.<sup>11</sup> From the definitions of the eigenfunctions in Eqs. (A2) and (A7), we find the following relations:

<sup>11</sup>The  $\mathbb{Z}_3^{(\text{ex})}$  singlet does not couple to the Wilson line phases in our model as discussed in Sec. VB, although the  $\mathbb{Z}_3^{(\text{ex})}$  triplets generally couple to the Wilson line phases as Eq. (A38).

$$\begin{aligned} g^{jk} \partial_{y^j} \partial_{y^k} \tilde{f}^{[p_s]}(\bar{y}^i N_i) &= \frac{2}{3} \sum_{\ell=1}^3 (\partial_{y^\ell})^2 \tilde{f}^{[p_s]}(\bar{y}^i N_i) \\ &= -\frac{2}{3R^2} \sum_{\ell=1}^3 (N_\ell)^2 \tilde{f}^{[p_s]}(\bar{y}^i N_i). \end{aligned} \quad (\text{A22})$$

Using them, we obtain the effective 4D Lagrangian  $\mathcal{L}_{\text{eff}}^{\text{singlet}}$  for  $\tilde{\phi}_{N_1, N_2}(x^\mu)$ :

$$\mathcal{L}_{\text{eff}}^{\text{singlet}} = - \iint_{T^2} d^2 y \phi^*(x^\mu, y^i) (\square - g^{jk} \partial_{y^j} \partial_{y^k}) \phi(x^\mu, y^i) \quad (\text{A23})$$

$$\begin{aligned} &= - \sum_{n_i \in \Lambda_{(\ell)}^{(p_t)}} \tilde{\phi}_{N_1, N_2}^* \left\{ \square + \frac{2}{3R^2} \sum_{k=1}^3 (N_k)^2 \right\} \tilde{\phi}_{N_1, N_2} \\ &- \tilde{\phi}_{0,0}^* \square \tilde{\phi}_{0,0} \delta_{p_t, 0} \delta_{p_s, 0}, \end{aligned} \quad (\text{A24})$$

where  $\tilde{\phi}_{N_1, N_2}(x^\mu)$  is an independent field for  $N_i \in \Lambda_{(\ell)}^{(p_t)}$  with a fixed  $\ell$ . Thus, the above KK mode is a canonically normalized 4D field with the following KK mass squared:

$$\begin{aligned} \frac{2}{3R^2} \sum_{k=1}^3 (N_k)^2 &= \frac{2}{3R^2} \left\{ \left(n_1 + \frac{p_t}{3}\right)^2 + \left(n_2 + \frac{p_t}{3}\right)^2 \right. \\ &\quad \left. + \left(-n_1 - n_2 - \frac{2p_t}{3}\right)^2 \right\} \end{aligned} \quad (\text{A25})$$

$$\begin{aligned} &= \frac{4}{3R^2} \left\{ \left(n_1 + \frac{p_t}{3}\right)^2 + \left(n_1 + \frac{p_t}{3}\right) \left(n_2 + \frac{p_t}{3}\right) \right. \\ &\quad \left. + \left(n_2 + \frac{p_t}{3}\right)^2 \right\}, \end{aligned} \quad (\text{A26})$$

which is the squared norm of the vector  $N/R$  on the momentum lattice spanned by  $\tilde{e}^i/R$ .

## 2. $\mathbb{Z}_3^{(\text{ex})}$ triplet fields

We start to study KK expansion of a  $\mathbb{Z}_3^{(\text{ex})}$  triplet field  $\phi^{(k)}$  that obeys the BCs as

$$\phi^{(k)}(\hat{T}_1[y^i]) = \omega^{p_t} \phi^{(k)}(y^i), \quad \phi^{(k)}(\hat{S}_0[y^i]) = \omega^{p_s} \phi^{(k+1)}(y^i), \quad (\text{A27})$$

where we have suppressed the coordinate  $x^\mu$  in the above for shorthand notations. Let us define  $\phi^{[p]}(y^i)$  as

$$\begin{aligned}\phi^{[p]}(y^i) &= \frac{1}{\sqrt{3}} \sum_{k=1}^3 \omega^{-kp} \phi^{(k)}(y^i), \\ \phi^{(k)}(y^i) &= \frac{1}{\sqrt{3}} \sum_{p=-1}^1 \omega^{kp} \phi^{[p]}(y^i).\end{aligned}\quad (\text{A28})$$

Then,  $\phi^{[p]}$  becomes an eigenstate of the BCs,

$$\phi^{[p]}(\hat{\mathcal{T}}_1[y^i]) = \omega^{p_s} \phi^{[p]}(y^i), \quad \phi^{[p]}(\hat{\mathcal{S}}_0[y^i]) = \omega^{p_s+p} \phi^{[p]}(y^i), \quad (\text{A29})$$

as the  $\mathbb{Z}_3^{(\text{ex})}$  singlet in Eq. (A1) but  $p_s$  is substituted by  $p_s + p$ . Thus, from a similar discussion deriving Eq. (A18), we define the KK expansion as

$$\phi^{[p]}(y^i) = \sum_{N \in \Lambda_{(\ell)}^{(p_i)}} \tilde{\phi}_{N_1, N_2}^{[p]} \tilde{f}^{[p_s+p]}(\bar{y}^i N_i) + \frac{\delta_{p,0} \delta_{p_s+p_0}}{2\pi R (\det g_{ij})^{1/4}} \tilde{\phi}_{0,0}^{[-p_s]}. \quad (\text{A30})$$

Using the above, we obtain the KK expansion of  $\phi^{(k)}(y^i)$  as

$$\begin{aligned}\phi^{(k)}(y^i) &= \frac{1}{\sqrt{3}} \sum_{N \in \Lambda_{(\ell)}^{(p_i)}} \sum_{p=-1}^1 \omega^{kp} \tilde{\phi}_{N_1, N_2}^{[p]} \tilde{f}^{[p_s+p]}(\bar{y}^i N_i) \\ &+ \frac{\omega^{-kp_s} \delta_{p,0}}{2\pi R (\det g_{ij})^{1/4}} \frac{\tilde{\phi}_{0,0}^{[-p_s]}}{\sqrt{3}}.\end{aligned}\quad (\text{A31})$$

Note that, as Eq. (A21), the KK mode  $\tilde{\phi}_{N_1, N_2}^{[p]}$  satisfy the following constraint:

$$\tilde{\phi}_{N_{1\pm\ell}, N_{2\pm\ell}}^{[p]} = \omega^{\mp\ell(p_s+p)} \tilde{\phi}_{N_1, N_2}^{[p]}. \quad (\text{A32})$$

In view of Eq. (A28), it is natural to define the KK mode  $\tilde{\phi}_{N_1, N_2}^{(k)}$  as

$$\tilde{\phi}_{N_1, N_2}^{(k)} \equiv \frac{1}{\sqrt{3}} \sum_{p=-1}^1 \omega^{kp} \tilde{\phi}_{N_1, N_2}^{[p]}, \quad \tilde{\phi}_{N_1, N_2}^{[p]} = \frac{1}{\sqrt{3}} \sum_{k=1}^3 \omega^{-kp} \tilde{\phi}_{N_1, N_2}^{(k)}. \quad (\text{A33})$$

As seen below,  $\tilde{\phi}_{N_1, N_2}^{(k)}$  is a basis that diagonalize contributions from the Wilson line phases to KK masses.

Combining Eq. (A31) and the second equation in (A33), we can expand  $\phi^{(k)}(y^i)$  by  $\tilde{\phi}_{N_1, N_2}^{(k)}$ . To see this, we use the formula

$$\frac{1}{\sqrt{3}} \sum_{p=-1}^1 \omega^{(k-k')p} \tilde{f}^{[p_s+p]}(\bar{y}^i N_i) = \omega^{-(k-k')p_s} f(\bar{y}^i N_{i+k-k'}), \quad (\text{A34})$$

derived from Eq. (A7). Using it, we obtain

$$\begin{aligned}\phi^{(k)}(y^i) &= \frac{1}{\sqrt{3}} \sum_{N \in \Lambda_{(\ell)}^{(p_i)}} \sum_{k'=1}^3 \omega^{-k'p_s} \tilde{\phi}_{N_1, N_2}^{(k-k')} f(\bar{y}^i N_{i+k'}) \\ &+ \frac{\omega^{-kp_s} \delta_{p,0}}{2\pi R (\det g_{ij})^{1/4}} \frac{\tilde{\phi}_{0,0}^{[-p_s]}}{\sqrt{3}}.\end{aligned}\quad (\text{A35})$$

From Eq. (A32), we find the constraint on  $\tilde{\phi}_{N_1, N_2}^{(k)}$  is written as

$$\tilde{\phi}_{N_{1\pm\ell}, N_{2\pm\ell}}^{(k)} = \omega^{\mp\ell p_s} \tilde{\phi}_{N_1, N_2}^{(k \mp \ell)}. \quad (\text{A36})$$

Let us derive the 4D effective Lagrangian for the triplet scalar defined in in Eq. (A27). We consider the 6D kinetic term,

$$\mathcal{L}_{\text{eff}}^{\text{triplet}} = - \iint_{T^2} d^2 y \sum_{k=1}^3 \phi^{(k)*}(y^i) (\square + \hat{M}_k^2) \phi^{(k)}(y^i), \quad (\text{A37})$$

where  $\hat{M}_k^2$  is a differential operator including Wilson line phases as in Eq. (5.9) and is defined by

$$\begin{aligned}\hat{M}_k^2 &= g^{ij} \left( -i\partial_{y^i} + \frac{\tilde{a}_{i+k}}{R} \right) \left( -i\partial_{y^j} + \frac{\tilde{a}_{j+k}}{R} \right) \\ &= \frac{2}{3} \sum_{\ell=1}^3 \left( -i\partial_{y^\ell} + \frac{\tilde{a}_{\ell+k}}{R} \right)^2.\end{aligned}\quad (\text{A38})$$

Using the KK expansion in Eq. (A35) and the definition of the eigenfunction in Eq. (A2), we obtain the effective 4D Lagrangian for  $\tilde{\phi}_{N_1, N_2}^{(k)}$  and the zero mode  $\tilde{\phi}_{0,0}^{[-p_s]}$  as

$$\mathcal{L}_{\text{eff}}^{\text{triplet}} = - \sum_{N \in \Lambda_{(\ell)}^{(p_i)}} \sum_{k=1}^3 \tilde{\phi}_{N_1, N_2}^{(k)*} \left\{ \square + \frac{2}{3R^2} \sum_{\ell=1}^3 (N_\ell + \tilde{a}_{\ell+k})^2 \right\} \tilde{\phi}_{N_1, N_2}^{(k)} - \delta_{p,0} \tilde{\phi}_{0,0}^{[-p_s]*} \left( \square + \frac{2}{3R^2} \sum_{\ell=1}^3 \tilde{a}_\ell^2 \right) \tilde{\phi}_{0,0}^{[-p_s]}, \quad (\text{A39})$$

where  $\tilde{\phi}_{N_1, N_2}^{(k)}$  is an independent and a canonically normalized fields for  $N_i \in \Lambda_{(\ell)}^{(p_i)}$  with a fixed  $\ell$ . With the help of Eq. (A36), we can rewrite Eq. (A39) with the summation over the dual lattice  $\Lambda^{(p_i)}$  as

$$\mathcal{L}_{\text{eff}}^{\text{triplet}} = - \sum_{N \in \Lambda^{(p_t)}} \tilde{\phi}_{N_1, N_2}^{(0)*} \left\{ \square + \frac{2}{3R^2} \sum_{\ell=1}^3 (N_\ell + \tilde{a}_\ell)^2 \right\} \tilde{\phi}_{N_1, N_2}^{(0)}, \quad (\text{A40})$$

where we have defined  $\tilde{\phi}_{0,0}^{(0)} \equiv \tilde{\phi}_{0,0}^{[-p_s]}$ . Although we choose  $k=0$  of  $\tilde{\phi}_{N_1, N_2}^{(k)}$  as a representative in the above, a similar expression holds for any choice of  $k$ . The KK mass in Eq. (A40) is again the squared norm of the vector as the case in Eq. (A26), but the vector  $N$  is shifted by the Wilson line phases as  $N + \tilde{a}_i \tilde{e}^i$ .

The KK mass spectrum in Eq. (A40) is a similar one in models with  $T^2$  compactification. This situation is shared with the  $S^1/\mathbb{Z}_2$  model with the diagonal embedding method, where the resulting KK mass spectrum is a similar one in models with  $S^1$  compactification.

## APPENDIX B: CALCULATION OF EFFECTIVE POTENTIALS ON $M^4 \times T^2/\mathbb{Z}_3$

We derive contributions from a  $\mathbb{Z}_3^{\text{(ex)}}$  triplet field to the effective potential obtained from the Lagrangian in Eq. (A37). For later convenience, we denote the KK mass in Eq. (A40) by

$$\begin{aligned} M^2(\tilde{a}_i) &\equiv \frac{2}{3R^2} \sum_{\ell=1}^3 (N_\ell + \tilde{a}_\ell)^2 \\ &= \frac{4}{3R^2} \{ (N_1 + \tilde{a}_1)^2 + (N_1 + \tilde{a}_1)(N_2 + \tilde{a}_2) \\ &\quad + (N_2 + \tilde{a}_2)^2 \}. \end{aligned} \quad (\text{B1})$$

In addition, we define  $\tilde{\mathbf{a}} = \tilde{a}_i \tilde{e}^i$ . Then, we can write  $M^2(\tilde{a}_i) = |\mathbf{N} + \tilde{\mathbf{a}}|^2/R^2$ . Since Eq. (A37) is rewritten as Eq. (A40), by performing the path integration of the KK modes  $\tilde{\phi}_{N_1, N_2}^{(0)}$ , we obtain the following contribution to the effective potential:

$$\Delta V^{(p_t)} \equiv \frac{\hat{N}_{\text{deg}}}{2} \sum_{N \in \Lambda^{(p_t)}} \int \frac{d^4 p_E}{(2\pi)^4} \ln(p_E^2 + M^2(\tilde{a}_i)), \quad (\text{B2})$$

where  $\hat{N}_{\text{deg}} = 2$  for the case of a complex scalar, and the square of an Euclidean four-momentum is denoted by  $p_E^2$ .

To deal with the divergent momentum integral, we use the zeta-function regularization and introduce

$$\zeta(s) \equiv \sum_{N \in \Lambda^{(p_t)}} \int \frac{d^4 p_E}{(2\pi)^4} (p_E^2 + M^2(\tilde{a}_i))^{-s}. \quad (\text{B3})$$

Then, the contributions to the potential is rewritten as

$$\Delta V^{(p_t)} = - \frac{\hat{N}_{\text{deg}}}{2} \lim_{s \rightarrow 0} \frac{d}{ds} \zeta(s). \quad (\text{B4})$$

A straightforward calculation shows

$$\zeta(s) = \frac{1}{8\pi^2} \sum_{N \in \Lambda^{(p_t)}} \int_0^\infty d\bar{p} \bar{p}^3 \int_0^\infty dt \frac{t^{s-1}}{\Gamma(s)} e^{-[\bar{p}^2 + M^2(\tilde{a}_i)]t} \quad (\text{B5})$$

$$= \frac{s}{16\pi^2} \sum_{N \in \Lambda^{(p_t)}} \int_0^\infty dt t^{-3} e^{-M^2(\tilde{a}_i)t} + \mathcal{O}(s^2), \quad (\text{B6})$$

where  $\Gamma(s)$  is the gamma function, and  $|s| \ll 1$  is implied. Thus, we get

$$\frac{d}{ds} \zeta(s) = \frac{1}{16\pi^2} \sum_{N \in \Lambda^{(p_t)}} \int_0^\infty dt t^{-3} e^{-M^2(\tilde{a}_i)t} + \mathcal{O}(s), \quad (\text{B7})$$

where the singularity associated with  $t \rightarrow 0$  corresponds to the ultraviolet divergence in the integral.

The  $\mathcal{O}(s^0)$  term in Eq. (B7) is evaluated by using the Poisson resummation formula, which is derived in the next section. In Eq. (C8), we set  $D=2$  and

$$\begin{aligned} d_i &= \frac{p_t}{3} + \tilde{a}_i, & A_{ij} &= \frac{\pi R^2}{t} g_{ij}, & (A^{-1})^{ij} &= \frac{t}{\pi R^2} g^{ij}, \\ \det A &= \frac{3\pi^2 R^4}{4t^2}, \end{aligned} \quad (\text{B8})$$

where  $g_{ij}$  and  $g^{ij}$  are the metric given in Sec. II. Let us introduce the vector  $\mathbf{w}$  and the lattice  $\Lambda_w$  expanded by  $\mathbf{e}_i$ , which is associated with the metric  $g_{ij}$ , as

$$\Lambda_w = \{ \mathbf{w} = w^1 \mathbf{e}_1 + w^2 \mathbf{e}_2 | w^1, w^2 \in \mathbb{Z} \}. \quad (\text{B9})$$

Then, we obtain

$$\begin{aligned} \sum_{N \in \Lambda^{(p_t)}} e^{-M^2(\tilde{a}_i)t} &= \sum_{N \in \Lambda^{(p_t)}} e^{-\frac{t}{R^2} |\mathbf{N} + \tilde{\mathbf{a}}|^2} \\ &= \frac{\sqrt{3}\pi R^2}{2\sqrt{t^2}} \sum_{\mathbf{w} \in \Lambda_w} e^{-\frac{\pi^2 R^2}{t} |\mathbf{w}|^2} e^{2\pi i \mathbf{w} \cdot \tilde{\mathbf{a}}'}, \end{aligned} \quad (\text{B10})$$

where we have defined  $\tilde{\mathbf{a}}' \equiv (p_t/3 + \tilde{a}_1) \tilde{\mathbf{e}}^1 + (p_t/3 + \tilde{a}_2) \tilde{\mathbf{e}}^2$  and

$$\begin{aligned} |\mathbf{w}|^2 &= (w^1)^2 + (w^2)^2 - w^1 w^2, \\ \mathbf{w} \cdot \tilde{\mathbf{a}}' &= (p_t/3 + \tilde{a}_1) w^1 + (p_t/3 + \tilde{a}_2) w^2. \end{aligned} \quad (\text{B11})$$

Thus, we can replace the summation over  $\Lambda^{(p_t)}$  by the summation over  $\Lambda_w$ . The integers  $w^i$  are often called winding numbers. Let us consider a continuum path on the covering space of  $T^2/\mathbb{Z}_3$ , where the separation between the endpoints of the path corresponds to the vector  $2\pi R \mathbf{w}$ . In this case, such continuum path represents a noncontractible cycle on  $T^2/\mathbb{Z}_3$ , whose winding number along the  $\mathbf{e}_i$  direction is given by  $w^i$ , except for the case of  $\mathbf{w} = 0$ .



This implies that the summation over the possible momentum states, i.e., KK modes, in the evaluation of the effective potential is replaced by performing the summation over the possible winding numbers. Notice that the term with  $\mathbf{w} = 0$  in the summation represents a local effect and is independent of the nonlocal Wilson line  $\tilde{a}_i$ . To deal with it, we define  $\Lambda'_w = \Lambda_w \setminus \{\mathbf{w} = 0\}$  and write  $\sum_{\mathbf{w} \in \Lambda_w} F(\mathbf{w}) = F(0) + \sum_{\mathbf{w} \in \Lambda'_w} F(\mathbf{w})$  for a function  $F(\mathbf{w})$ .

From the above, we find

$$\begin{aligned} \lim_{s \rightarrow 0} \frac{d}{ds} \zeta(s) &= \frac{\sqrt{3}}{16\pi^7 R^4} \sum_{\mathbf{w} \in \Lambda'_w} \frac{e^{2\pi i \mathbf{w} \cdot \tilde{\mathbf{a}}'}}{(|\mathbf{w}|^2)^3} + (\text{const}) \\ &= \frac{\sqrt{3}}{16\pi^7 R^4} \sum_{\mathbf{w} \in \Lambda'_w} \frac{\cos(2\pi \mathbf{w} \cdot \tilde{\mathbf{a}}')}{(|\mathbf{w}|^2)^3} + (\text{const}). \end{aligned} \quad (\text{B12})$$

In the last equation, we have used that  $|\mathbf{w}|^2$  is symmetric under  $w^i \rightarrow -w^i$ . We have separated the irrelevant constant term with  $\mathbf{w} = 0$  in the above. In this paper, we discard the constant term in the effective potential. The summation over all integers for  $w^1$  and  $w^2$  except for  $(w^1, w^2) = (0, 0)$  is denoted by  $w^1, w^2 \in \mathbb{Z}'$ . Finally, we obtain

$$\Delta V(\tilde{a}_i) = \hat{N}_{\text{deg}} \mathcal{V}^{(p_i)}(\tilde{a}_i), \quad (\text{B13})$$

$$\begin{aligned} \mathcal{V}^{(p_i)}(\tilde{a}_i) &\equiv -\frac{\sqrt{3}}{32\pi^7 R^4} \sum_{w^1, w^2 \in \mathbb{Z}'} \\ &\times \frac{\cos(2\pi[w^1(p_i/3 + \tilde{a}_1) + w^2(p_i/3 + \tilde{a}_2)])}{[(w^1)^2 - w^1 w^2 + (w^2)^2]^3}. \end{aligned} \quad (\text{B14})$$

### APPENDIX C: THE POISSON RESUMMATION FORMULA IN $D$ DIMENSIONS

Let us consider the summation including a matrix  $A^{-1}$ , which is the inverse of a symmetric  $D \times D$  matrix  $A$ , as

$$I_D = \sum_{n_1, \dots, n_D \in \mathbb{Z}} e^{-\pi(n_i + d_i)(A^{-1})^{ij}(n_j + d_j)}, \quad (\text{C1})$$

where  $(A^{-1})^{ij}$  are elements of  $A^{-1}$ , and the indices  $i, j$  run from 1 to  $D$ . Since  $I_D$  is periodic under  $d_i \rightarrow d_i + 1$ , we can expand it as

$$\begin{aligned} I_D &= \sum_{w^1, \dots, w^D \in \mathbb{Z}} C(w^i) e^{2\pi i w^i d_i}, \quad \text{where} \\ C(w^i) &= \left( \prod_{i=1}^D \int_0^1 d\tilde{a}_i \right) e^{-2\pi i w^j \tilde{a}_j} I_D. \end{aligned} \quad (\text{C2})$$

Introducing  $\beta_i = n_i + d_i$ , we rewrite  $C(w^i)$  as

$$\begin{aligned} C(w^i) &= \left( \prod_{i=1}^D \int_{-\infty}^{\infty} d\beta_i \right) e^{-\pi \beta_j (A^{-1})^{jk} \beta_k} e^{-2\pi i w^l \beta_l} \\ &= \left( \prod_{i=1}^D \int_{-\infty}^{\infty} d\tilde{\beta}_i \right) e^{-\pi \tilde{\beta}_j (A^{-1})^{jk} \tilde{\beta}_k} e^{-\pi w^j A_{jk} w^k}, \end{aligned} \quad (\text{C3})$$

where  $\tilde{\beta}_j = \beta_j + i A_{jk} w^k$ .

Since  $A$  is symmetric,  $A^{-1}$  is diagonalized by an orthogonal matrix  $O$  ( $OO^T = 1$ ) and is written as

$$(A^{-1})^{ij} = (O^T \hat{A}^{-1} O)^{ij}, \quad (\hat{A}^{-1})^{kl} = (a^{-1})^k \delta^{kl}, \quad (\text{C4})$$

where  $\hat{A}^{-1}$  is the diagonal matrix and  $(a^{-1})^k$  is a  $k$ -th eigenvalue of  $\hat{A}^{-1}$ . Defining  $z_i = O_i^j \tilde{\beta}_j$ , we obtain

$$C(w^i) = \left( \prod_{i=1}^D \int_{\mathcal{C}_i} dz_i e^{-\pi(a^{-1})^i(z_i)^2} \right) e^{-\pi w^j A_{jk} w^k}, \quad (\text{C5})$$

where  $\mathcal{C}_i$  denotes a path in the complex plane defined by  $\text{Re}(z_i) = (-\infty, \infty)$  with a fixed  $\text{Im}(z_i) = O_i^j A_{jk} w^k$ . With the help of the relation

$$\int_{-\infty}^{\infty} dx e^{-\pi c(x+iy)^2} = \int_{-\infty}^{\infty} dx e^{-\pi c x^2} = \frac{1}{\sqrt{c}}, \quad (\text{C6})$$

we obtain

$$C(w^i) = \left( \prod_{i=1}^D \frac{1}{\sqrt{(a^{-1})^i}} \right) e^{-\pi w^j A_{jk} w^k} = \sqrt{\det A} e^{-\pi w^j A_{ij} w^j}. \quad (\text{C7})$$

Thus, the following relation holds:

$$\begin{aligned} &\sum_{n_1, \dots, n_D \in \mathbb{Z}} e^{-\pi(n_i + d_i)(A^{-1})^{ij}(n_j + d_j)} \\ &= \sqrt{\det A} \sum_{w^1, \dots, w^D \in \mathbb{Z}} e^{-\pi w^j A_{ij} w^j} e^{2\pi i w^k d_k}, \end{aligned} \quad (\text{C8})$$

which is the Poisson resummation formula used in Appendix B. The above is naturally rewritten by the vectors and the metric that are defined by  $\mathbf{W} = w^i \mathbf{E}_i$ ,  $\mathbf{n} = n_i \tilde{\mathbf{E}}^i$ ,  $\mathbf{d} = d_i \tilde{\mathbf{E}}^i$ ,  $\mathbf{E}_i \cdot \tilde{\mathbf{E}}^j = \delta_i^j$ , and  $\mathbf{E}_i \cdot \mathbf{E}_j = A_{ij}$  as

$$\sum_{n_1, \dots, n_D \in \mathbb{Z}} e^{-\pi|\mathbf{n} + \mathbf{d}|^2} = \sqrt{\det A} \sum_{w^1, \dots, w^D \in \mathbb{Z}} e^{-\pi|\mathbf{W}|^2} e^{2\pi i \mathbf{W} \cdot \mathbf{d}}. \quad (\text{C9})$$

### APPENDIX D: FERMION FIELDS IN SIX DIMENSIONS

We here summarize the notations related to fermion fields in 6D theories. First, we work with the metric  $\eta_{MN} = \text{diag}(1, -1, -1, -1, -1, -1)$ . The 4D gamma matrices  $\gamma^\mu$  can be written by

$$\begin{aligned}\gamma^\mu &= \begin{pmatrix} 0 & \sigma^\mu \\ \bar{\sigma}^\mu & 0 \end{pmatrix}, & \sigma^\mu &= (I_2, \sigma^1, \sigma^2, \sigma^3), \\ \bar{\sigma}^\mu &= (I_2, -\sigma^1, -\sigma^2, -\sigma^3),\end{aligned}\quad (\text{D1})$$

where  $I_2$  is the  $2 \times 2$  identity matrix and  $\sigma^i$  ( $i = 1, 2, 3$ ) are the Pauli matrices. A 4D Dirac fermion  $\psi$  is denoted by  $\psi = \psi_L + \psi_R$ , where 4D chirality is defined by

$$\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} -I_2 & 0 \\ 0 & I_2 \end{pmatrix}, \quad \gamma_5\psi_L = -\psi_L, \quad \gamma_5\psi_R = \psi_R. \quad (\text{D2})$$

Thus, the 4D Weyl fermions are written by

$$\psi_L = \begin{pmatrix} \xi_L \\ 0 \end{pmatrix}, \quad \psi_R = \begin{pmatrix} 0 \\ \bar{\eta}_R \end{pmatrix}, \quad (\text{D3})$$

where  $\xi_L$  and  $\bar{\eta}_R$  are two-component spinors.

The 6D gamma matrices can be defined by the 4D gamma matrices in Eq. (D1) as

$$\begin{aligned}\Gamma^\mu &= \sigma^3 \otimes \gamma^\mu = \begin{pmatrix} \gamma^\mu & 0 \\ 0 & -\gamma^\mu \end{pmatrix}, & \Gamma^5 &= i\sigma^1 \otimes I_4 = \begin{pmatrix} 0 & iI_4 \\ iI_4 & 0 \end{pmatrix}, \\ \Gamma^6 &= i\sigma^2 \otimes I_4 = \begin{pmatrix} 0 & I_4 \\ -I_4 & 0 \end{pmatrix},\end{aligned}\quad (\text{D4})$$

so that they satisfy the 6D Clifford algebra,

$$\{\Gamma^M, \Gamma^N\} = 2\eta^{MN}. \quad (\text{D5})$$

To study the 6D chirality, it is useful to define

$$\begin{aligned}\Gamma_7 &= \Gamma^0\Gamma^1\Gamma^2\Gamma^3\Gamma^5\Gamma^6 = -\sigma^3 \otimes \gamma_5 \\ &= \begin{pmatrix} -\gamma_5 & 0 \\ 0 & \gamma_5 \end{pmatrix} = \text{diag}(1, 1, -1, -1, -1, -1, 1, 1),\end{aligned}\quad (\text{D6})$$

which satisfies  $\{\Gamma_7, \Gamma^M\} = 0$ . The 6D Dirac fermion  $\Psi$  is decomposed into a sum of the 6D Weyl fermions  $\Psi_\pm$ , which are eigenstates of  $\Gamma_7$ , as

$$\Psi = \Psi^+ + \Psi^-, \quad \Gamma_7\Psi^\pm = \pm\Psi^\pm. \quad (\text{D7})$$

Thus, we can write

$$\begin{aligned}\Psi^\pm &\equiv \frac{1 \pm \Gamma_7}{2}\Psi = \begin{pmatrix} \frac{1 \pm \gamma_5}{2} & 0 \\ 0 & \frac{1 \pm \gamma_5}{2} \end{pmatrix}\Psi, & \Psi^+ &= \begin{pmatrix} \psi_L^+ \\ \psi_R^+ \end{pmatrix}, \\ \Psi^- &= \begin{pmatrix} \psi_R^- \\ \psi_L^- \end{pmatrix}.\end{aligned}\quad (\text{D8})$$

A 6D Weyl fermion  $\Psi^\pm$  involves a vectorlike pair of 4D Weyl fermions. By using the two-component spinor notation in Eq. (D3), we can also write

$$\Psi = \Psi^+ + \Psi^- = \begin{pmatrix} \psi_L^+ + \psi_R^- \\ \psi_R^+ + \psi_L^- \end{pmatrix} = \begin{pmatrix} \xi_L^+ \\ \bar{\eta}_R^- \\ \xi_L^- \\ \bar{\eta}_R^+ \end{pmatrix}. \quad (\text{D9})$$

Let us study fermion bilinears. We define  $\bar{\Psi} \equiv \Psi^\dagger\Gamma^0$  and find

$$\bar{\Psi}^+ = (\bar{\psi}_L^+, -\bar{\psi}_R^+), \quad \bar{\Psi}^- = (\bar{\psi}_R^-, -\bar{\psi}_L^-). \quad (\text{D10})$$

The fermion bilinears without derivatives are given by

$$\bar{\Psi}\Psi = \bar{\Psi}^-\Psi^+ + \bar{\Psi}^+\Psi^-, \quad (\text{D11})$$

which are written in terms of the 4D Weyl fermions as

$$\bar{\Psi}^-\Psi^+ = \bar{\psi}_R^-\psi_L^+ - \bar{\psi}_L^-\psi_R^+, \quad \bar{\Psi}^+\Psi^- = \bar{\psi}_L^+\psi_R^- - \bar{\psi}_R^+\psi_L^-. \quad (\text{D12})$$

To obtain the kinetic terms for fermion fields, we use the fermion bilinears with a derivative,

$$\bar{\Psi}\Gamma^M\partial_M\Psi = \bar{\Psi}^+\Gamma^M\partial_M\Psi^+ + \bar{\Psi}^-\Gamma^M\partial_M\Psi^-, \quad (\text{D13})$$

where

$$\Gamma^M\partial_M = \begin{pmatrix} \gamma^\mu\partial_\mu & i(\partial_5 - i\partial_6) \\ i(\partial_5 + i\partial_6) & -\gamma^\mu\partial_\mu \end{pmatrix}. \quad (\text{D14})$$

Thus, by using the 4D Weyl fermions, we can rewrite the above as

$$\begin{aligned}\bar{\Psi}^+\Gamma^M\partial_M\Psi^+ &= \bar{\psi}_L^+\gamma^\mu\partial_\mu\psi_L^+ + \bar{\psi}_R^+\gamma^\mu\partial_\mu\psi_R^+ \\ &\quad + \bar{\psi}_L^+i(\partial_5 - i\partial_6)\psi_R^+ - \bar{\psi}_R^+i(\partial_5 + i\partial_6)\psi_L^+, \end{aligned}\quad (\text{D15})$$

$$\begin{aligned}\bar{\Psi}^-\Gamma^M\partial_M\Psi^- &= \bar{\psi}_L^-\gamma^\mu\partial_\mu\psi_L^- + \bar{\psi}_R^-\gamma^\mu\partial_\mu\psi_R^- \\ &\quad + \bar{\psi}_R^-i(\partial_5 - i\partial_6)\psi_L^- - \bar{\psi}_L^-i(\partial_5 + i\partial_6)\psi_R^-. \end{aligned}\quad (\text{D16})$$

The mixing terms between  $\psi_L^\pm$  and  $\psi_R^\pm$  include the derivatives on the extradimensional coordinates.

To deal with the gamma matrices and study fermion fields on  $M^4 \times T^2/\mathbb{Z}_3$ , it is useful to introduce the oblique coordinates discussed in Sec. II. With the oblique coordinates  $y^1$  and  $y^2$  found in Eq. (2.2), we naturally define the new gamma matrices from  $\Gamma^5$  and  $\Gamma^6$  as

$$\begin{aligned}\Gamma^{y^1} &\equiv \Gamma^5 + \frac{1}{\sqrt{3}}\Gamma^6 = \frac{2}{\sqrt{3}} \begin{pmatrix} 0 & -\bar{\omega} \\ \omega & 0 \end{pmatrix} \otimes I_4, \\ \Gamma^{y^2} &\equiv \frac{2}{\sqrt{3}}\Gamma^6 = \frac{2}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes I_4.\end{aligned}\quad (\text{D17})$$

As expected, they satisfy

$$\{\Gamma^{y^i}, \Gamma^{y^j}\} = -2g^{ij}, \quad \{\Gamma^\mu, \Gamma^{y^i}\} = 0, \quad (\text{D18})$$

where  $g^{ij}$  is the metric in Eq. (2.16). It is also natural to define  $\Gamma_{y^i} \equiv -g_{ij}\Gamma^{y^j}$ , which are explicitly written as

$$\Gamma_{y^1} = -i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes I_4, \quad \Gamma_{y^2} = -i \begin{pmatrix} 0 & \bar{\omega} \\ \omega & 0 \end{pmatrix} \otimes I_4. \quad (\text{D19})$$

We also introduce the useful notations:

$$\Gamma_{y^3} = -\Gamma_{y^1} - \Gamma_{y^2} = -i \begin{pmatrix} 0 & \omega \\ \bar{\omega} & 0 \end{pmatrix} \otimes I_4, \quad \Gamma_{y^{i+3}} = \Gamma_{y^i}. \quad (\text{D20})$$

Then, Eq. (D14) is rewritten as

$$\begin{aligned}\Gamma^M \partial_M &= \Gamma^\mu \partial_\mu - g^{ij} \Gamma_{y^i} \partial_{y^j} = \Gamma^\mu \partial_\mu - \frac{2}{3} \sum_{\ell=1}^3 \Gamma_{y^\ell} \partial_{y^\ell} \\ &= \begin{pmatrix} \gamma^\mu \partial_\mu & i\frac{2}{3}(\partial_{y^1} + \bar{\omega} \partial_{y^2} + \omega \partial_{y^3}) \\ i\frac{2}{3}(\partial_{y^1} + \omega \partial_{y^2} + \bar{\omega} \partial_{y^3}) & -\gamma^\mu \partial_\mu \end{pmatrix}.\end{aligned}\quad (\text{D22})$$

Let us discuss the BC on  $T^2/\mathbb{Z}_3$  related to the  $\mathbb{Z}_3$  transformation  $y^i \rightarrow \hat{S}_0[y^i]$  for fermion fields. The  $\mathbb{Z}_3$  transformation generated by  $\hat{S}_0$  is a  $SO(2) \cong U(1)$  rotation with the angle  $2\pi/3$  on a two-dimensional Euclidean space, under which the derivative  $\partial_{y^i}$  transforms to  $\partial_{y^{i+1}}$  as in Eq. (2.19). It is convenient to define a matrix  $\tilde{S}_\Psi$  that satisfies

$$\tilde{S}_\Psi^\dagger \Gamma_{y^i} \tilde{S}_\Psi = \Gamma_{y^{i+1}}, \quad [\Gamma^\mu, \tilde{S}_\Psi] = 0, \quad \tilde{S}_\Psi^\dagger \tilde{S}_\Psi = I_2 \otimes I_4. \quad (\text{D23})$$

One of the possible choices is

$$\tilde{S}_\Psi \equiv - \begin{pmatrix} \omega & 0 \\ 0 & \bar{\omega} \end{pmatrix} \otimes I_4. \quad (\text{D24})$$

Using  $\tilde{S}_\Psi$ , we can define the transformation law of the 6D Dirac fermion  $\Psi$  under the  $SO(2)$  rotation with the angle  $2\pi/3$  as  $\Psi \rightarrow \tilde{S}_\Psi \Psi$  so that the  $2\pi$  rotation gives  $\Psi \rightarrow -\Psi$ . One sees that the  $2\pi/3$  rotation keeps the fermion bilinear in Eq. (D13) invariant as required from the 6D Lorentz invariance, with the help of the relation

$$\tilde{S}_\Psi^\dagger \Gamma^0 \Gamma^M \partial_M \tilde{S}_\Psi = \tilde{S}_\Psi^\dagger \Gamma^0 \left( \Gamma^\mu \partial_\mu - \frac{2}{3} \sum_{\ell=1}^3 \Gamma_{y^\ell} \partial_{y^\ell} \right) \tilde{S}_\Psi \quad (\text{D25})$$

$$= \Gamma^0 \left( \Gamma^\mu \partial_\mu - \frac{2}{3} \sum_{\ell=1}^3 \Gamma_{y^{\ell-1}} \partial_{y^{\ell-1}} \right) = \Gamma^0 \Gamma^M \partial_M. \quad (\text{D26})$$

We can define the BC for the 6D Dirac fermion  $\Psi(x^\mu, y^i)$  as

$$\Psi(x^\mu, \hat{S}_0[y^i]) = -\omega^{p_s} \tilde{S}_\Psi \Psi(x^\mu, y^i), \quad (\text{D27})$$

where  $p_s \in \{0, \pm 1\}$  can be chosen by hand, and the overall minus sign on the right-hand side originates from the fermion number operator. We note that the BC in Eq. (D27) is consistent with  $\hat{S}_0^3 = \hat{I}$  as required. Using the 4D Weyl fermions, we rewrite the BC as follows:

$$\begin{aligned}\psi_L^\pm(x^\mu, \hat{S}_0[y^i]) &= \omega^{p_s \pm 1} \psi_L^\pm(x^\mu, y^i), \\ \psi_R^\pm(x^\mu, \hat{S}_0[y^i]) &= \omega^{p_s \mp 1} \psi_R^\pm(x^\mu, y^i),\end{aligned}\quad (\text{D28})$$

which allows us to leave a 4D chiral fermion spectrum as the zero mode from a 6D Weyl fermion  $\Psi^\pm$ .

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