

**Majorana fermions and  $CP$  violation from 5-dimensional theories: A systematic approach**

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Within five-dimensional compactified theories we discuss generalized periodicity and orbifold boundary conditions that allow for mixing between particles and antiparticles after a shift by the size of extra dimensions or after the orbifold reflection. A systematic strategy for constructing 4-dimensional models is presented, in particular, we find a general form of the periodicity and orbifold conditions that are allowed by consistency requirements. We formulate general conditions for a presence of massless Kaluza-Klein modes and discuss remaining gauge symmetry of the zero-mode sector. It is shown that if the orbifold twist operation transforms particles into antiparticles then the zero-mode fermions are 4-dimensional Majorana fermions. The possibility of explicit and spontaneous  $CP$  violation is discussed. General considerations are illustrated by many Abelian and non-Abelian examples.

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**I. INTRODUCTION**

In the standard model (SM), the Higgs mechanism is responsible for generation of fermion and vector-boson masses. This mechanism, though it leads to renormalizable and unitary theories, has severe naturalness problems associated with the so-called “hierarchy problem” [1]. The tree-level version of this problem reduces to the fact that a possible (and in the context of grand unified theories even necessary) huge ratio of mass scales is adopted without any explanation (aside from a desire to make these models phenomenologically viable). Radiative corrections usually exacerbate this problem as the quadratic corrections to the scalar masses tend to destabilize the original ratio, which requires order-by-order fine tuning of the parameters.

Extra dimensional extensions of the SM offer a novel approach to the gauge symmetry breaking in which the hierarchy problem could be either solved or at least reformulated in terms of geometry of the higher-dimensional space. Among various attempts in this direction it is worth mentioning the following:

- (i) The spontaneous breaking of gauge symmetries by imposing nontrivial boundary conditions along the extra (compactified) dimensions; the so-called Scherk-Schwarz (SS) mechanism [2].
- (ii) Symmetry breaking through a nonzero vacuum expectation value of extra components of the higher-dimensional gauge fields; the Hosotani mechanism [3].<sup>1</sup>

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<sup>1</sup>If the symmetry to be broken is a local one, then the Hosotani mechanism is equivalent to the Scherk-Schwarz breaking, see e.g. [4].

- (iii) Gauge symmetry braking by asymmetric boundary conditions (BC) in models of extra dimensions compactified on an interval [5].

It is worth noting that even though 5D gauge theories are nonrenormalizable, nevertheless, as is has been recently verified [6], the effective 4-dimensional (4D) theories are tree-level unitary.

In a recent publication [7] we have shown that 5D quantum electrodynamics compactified on a circle violates  $CP$  either explicitly through a nonsymmetric BC or, what is theoretically much more appealing, spontaneously through a nonzero one-loop vacuum expectation value for the zero Kaluza-Klein (KK) mode of the extra component of the  $U(1)$  gauge field. The implementation of this idea in a realistic model of  $CP$  violation (CPV) based on a 5D theory requires that the theory produce the correct chiral and flavor structures in the light sector. We consider this latter issue in this paper.

In order to produce a chiral effective 4D theory we will follow a standard approach and consider a 5-dimensional gauge theory compactified on the  $S_1/Z_2$  orbifold. We will, however, modify and generalize the usual treatment by allowing nonstandard twist operations. Specifically ( $y$  denotes the coordinate of  $S_1/Z_2$  and  $L$  the radius of  $S_1$ ) under the translation  $y \rightarrow y + L$ , or under orbifold  $Z_2$  reflection  $y \rightarrow -y$  we will allow mixing between particles and their charge-conjugated counterparts. Such mixing offers a particularly useful way to construct models that generate spontaneous CPV in the same spirit as in [7]; theories of this type are characterized by a nonstandard orbifold parity for the fifth component of the gauge field, as only then the corresponding zero mode survives, and it is the vacuum expectation value of this zero mode that is responsible for CPV. In this case, however the corresponding 4D compo-

nents *do not* have a zero mode, and this corresponds to a reduction of the light-sector gauge group. We show below that this situation is indeed realized when nontrivial orbifold boundary conditions are chosen.

Allowing the boundary conditions to mix particles and antiparticles often reduces by one half the fermionic degrees of freedom and the surviving KK modes (including zero modes) behave as 4D Majorana fermions. Such a mechanism will be described below and will be of use when constructing models for neutrino physics within the context of higher-dimensional theories

The paper is organized as follows. In Sec. II we fix our notation and we consider the basic properties of the 5D theory including gauge symmetry and discrete symmetries. Section V contains discussion of zero-mode sector with general conditions which must be satisfied for the existence of zero modes. In Sec. III we illustrate the general discussion within Abelian theories containing one or two fermionic fields. Section IV shows non-Abelian examples of models with the generalized BC. Summary and conclusions are presented in Sec. VI. The appendix contains a detailed discussion of the single Abelian fermion and of the possibility for the spontaneous CPV.

## II. GENERAL CONSIDERATIONS

### A. The Lagrangian

We will consider a general 5-dimensional (5D) gauge theory with the gauge fields  $A_M$  coupled to a fermionic multiplet  $\Psi$ . The corresponding Lagrangian takes the form

$$\mathcal{L} = -\frac{1}{4} \sum_a \frac{1}{g_a^2} F_{MN}^a F^{aMN} + \bar{\Psi} (i\gamma^N D_N - M) \Psi, \quad (1)$$

where  $D_N = \partial_N + ig_5 A_N$ ,  $A_N = A_N^a T^a$ . We assume a general gauge group (not necessarily simple), where the gauge couplings are all expressed in units of  $g_5$  (which proves convenient since these couplings are not dimensionless) and are absorbed in the definition of the gauge fields; the group generators  $T_a$  are assumed to be Hermitian. All fermions are collected in the multiplet  $\Psi$  that is in general reducible, and may contain several submultiplets transforming according to the same gauge-group irreducible representation<sup>2</sup>. We will allow all fields to propagate throughout the 5D manifold.

We assume that the global topology of the 5-dimensional space-time is  $\mathbb{M}^4 \times (S_1/Z_2)$ . We denote by  $x^\mu$ ,  $\mu = 0, \dots, 4$  the  $\mathbb{M}^4$  coordinates (with  $x^0$  the only timelike

<sup>2</sup>We could, in principle, consider a nonstandard kinetic term,  $\bar{\psi} Z \gamma^N \partial_N \psi$ , with  $Z$  a Hermitian matrix. However, if we restrict ourselves to nontachyonic theories, then the eigenvalues of  $Z$  must be positive, so in the diagonal basis we have  $Z = K^2$ , where  $K$  is a real diagonal matrix. The rescaling  $\psi \rightarrow K^{-1} \psi$  would bring the kinetic term to its standard canonical form adopted in (1).

direction); and by  $y$  that of  $S_1/Z_2$ , with  $0 \leq y \leq L$  and  $y$  identified with  $-y$ . The metric is assumed to be flat, with convention  $g_{NM} = \text{diag}(1, -1, -1, -1, -1)$  with the last entry associated with  $S_1/Z_2$ .

Given this space-time structure the fields can have nontrivial boundary conditions (BC) in the  $y$  coordinate, both under translations  $y \rightarrow y + L$  and inversions  $y \rightarrow -y$ . We will consider the most general boundary conditions allowed by the gauge and Lorentz (in  $\mathbb{M}^4$ ) symmetries, which may involve both the fields and their charge conjugates. Such mixed BC can violate some of the global symmetries, and the conditions under which this occurs and its consequences will be investigated below. It is worth emphasizing that the theory is defined by (1) together with the imposed BC, all of which we assume fixed.

In order to simplify our notation we will often suppress the dependence of fields on  $x$ , and write e.g.  $\chi(y)$  or  $A_M(y)$  instead of  $\chi(x, y)$  and  $A_M(x, y)$ , respectively; it should be understood that whenever a field depends on  $y$  it is also a function of  $x$ .

### B. Periodicity

As mentioned above we will discuss generalized periodicity conditions that allow mixing between particles and antiparticles:

$$\begin{aligned} \Psi_{L/R}(y + L) &= \Gamma_{L/R} \Psi_{L/R}(y) + Y_{L/R}^* \Psi_{L/R}^c(y), \\ A_N(y + L) &= \begin{cases} +U_1^\dagger A_N(y) U_1 & (P1), \\ -U_2^\dagger A_N^T(y) U_2 & (P2), \end{cases} \end{aligned} \quad (2)$$

where  $\Psi^c$  denotes the charged-conjugate field  $C_5(\bar{\psi})^T$  with  $C_5$  the 5D charge conjugation operator defined by the relation  $\gamma_0^* C_5^\dagger \gamma_0 \gamma_N C_5 = \gamma_N^T$ ,<sup>3</sup>  $U_{1,2}$  are global elements of the gauge group while the matrices  $\Gamma$  and  $Y$  are matrices constrained by requiring invariance of  $\mathcal{L}$  under the so-called twist operation defined by the right-hand side of (2). In particular, it is easy to see that the invariance of the fermionic kinetic term  $\bar{\Psi} i \gamma^N \partial_N \Psi$  requires  $\Gamma_L = \Gamma_R = \Gamma$  and  $Y_L = Y_R = Y$ . Therefore we will consider only the nonchiral BC  $\Psi(y + L) = \Gamma \Psi(y) + Y^* \Psi^c(y)$ . Note that the matrices  $\Gamma$  and  $Y$  in general affect both flavor and gauge indices.

The motivation for considering the option  $P2$  is to allow for the presence of the charge-conjugate gauge fields in the BC in parallel with our choice of fermionic boundary conditions, which also involve charge-conjugate fields. It

<sup>3</sup>Whenever an explicit representation is needed for the Dirac matrices we will adopt the Dirac representation. In this case  $C_5 = \gamma_1 \gamma_3$ . The 5D parity, which will be relevant later, is defined by  $\Psi \rightarrow P \Psi$  with  $P = \gamma_0 \gamma_4$ . We also choose  $i \gamma^4 = +\gamma_5 = i \gamma^0 \gamma^1 \gamma^2 \gamma^3$ . Note that in 5D, the parity reflection is defined [8] such that one spatial component is preserved:  $x^{0,4} \rightarrow x^{0,4}$  and  $x^i \rightarrow -x^i$ , for  $i = 1, 2, 3$ .

should be emphasized that a linear combination of  $P1$  and  $P2$  is not allowed since it does not leave the gauge-kinetic term invariant.<sup>4</sup>

In describing the constraints imposed by the invariance of  $\mathcal{L}$  under (2) it proves convenient to introduce the following notation:

$$\begin{aligned} \chi &\equiv \begin{pmatrix} \Psi^c \\ \Psi \end{pmatrix}, & \mathcal{A} &\equiv \begin{pmatrix} \Gamma & -Y^* \\ Y & \Gamma^* \end{pmatrix}, \\ \tau^a &\equiv \begin{pmatrix} T_a & 0 \\ 0 & -T_a^* \end{pmatrix}, & \mathcal{U}_1 &\equiv \begin{pmatrix} U_1 & 0 \\ 0 & U_1^* \end{pmatrix}, \\ & & \mathcal{U}_2 &\equiv \begin{pmatrix} 0 & U_2^* \\ U_2 & 0 \end{pmatrix}, \end{aligned} \quad (3)$$

in terms of which the fermionic periodicity conditions are simply

$$\chi(y+L) = \mathcal{A}^* \chi(y). \quad (4)$$

Requiring invariance of the kinetic term  $\bar{\Psi} i \gamma^N D_N \Psi$  gives the following conditions on the acceptable BC:

$$\mathcal{A}^\dagger \mathcal{A} = 1, \quad \begin{aligned} P1: & [\tau_a, \mathcal{U}_1 \mathcal{A}] = 0, \\ P2: & [\tau_a, \mathcal{U}_2 \mathcal{A}] = 0. \end{aligned} \quad (5)$$

Decomposing  $\Psi$  into a set of gauge multiplets  $\{\psi_r\}$  each transforming as an irreducible representation of the gauge group, we find that  $\mathcal{A}$  can mix  $\psi_r$  with  $\psi_s$  (via  $\Gamma$ ) or with  $\psi_u^c$  (via  $Y$ ) provided  $\psi_s$  and  $\psi_u^c$  belong to the same irreducible representation as  $\psi_r$ . We will discuss this in detail in Sec. II F.

The conditions for the mass term to be invariant under the twist operation can be derived in the same way, we find

$$[\mathcal{A}, \mathcal{M}] = 0; \quad \mathcal{M} \equiv \begin{pmatrix} M & 0 \\ 0 & -M^* \end{pmatrix}. \quad (6)$$

We note that it is possible to choose a basis where the fermion fields are simply periodic: writing  $\mathcal{A}^* = e^{i\mathcal{K}}$ , the fields (see also [9]):

$$\chi'(y) = e^{-i\mathcal{K}y/L} \chi \quad (7)$$

satisfy  $\chi'(y+L) = \chi'(y)$ . Such a transformation, however, generates a nonstandard  $y$  and  $\mathcal{A}$ -dependent mass term. We do not use the above field redefinition because of this complication.

### C. Orbifold reflections

In a similar way we adopt the most general twist transformation for the orbifold reflection  $y \rightarrow -y$ . The BC read

<sup>4</sup>For Abelian groups there appears to be an additional sign freedom since the gauge-kinetic term is even in  $A$ . One can verify, however, that this is in fact covered by either  $P1$  or  $P2$ .

$$\begin{aligned} \chi(-y) &= \gamma_5 \mathcal{B}^* \chi(y) \\ A_N(-y) &= \begin{cases} (-1)^{s_N} \tilde{U}_1^\dagger A_N(y) \tilde{U}_1 & (R1), \\ (-1)^{1-s_N} \tilde{U}_2^\dagger A_N^T(y) \tilde{U}_2 & (R2), \end{cases} \end{aligned} \quad (8)$$

where  $s_N = \delta_{N,4}$ ,  $\tilde{U}_{1,2}$  are global gauge transformations and

$$\mathcal{B} \equiv \begin{pmatrix} -\tilde{\Gamma} & \tilde{Y}^* \\ \tilde{Y} & \tilde{\Gamma}^* \end{pmatrix}. \quad (9)$$

Requiring now the invariance of  $\mathcal{L}$  under (8) implies

$$\mathcal{B}^\dagger \mathcal{B} = 1, \quad \begin{aligned} R1: & [\tau_a, \tilde{U}_1 \mathcal{B}] = 0, \\ R2: & [\tau_a, \tilde{U}_2 \mathcal{B}] = 0, \end{aligned} \quad (10)$$

where

$$\tilde{U}_1 \equiv \begin{pmatrix} \tilde{U}_1 & 0 \\ 0 & \tilde{U}_1^* \end{pmatrix}, \quad \tilde{U}_2 \equiv \begin{pmatrix} 0 & \tilde{U}_2^* \\ \tilde{U}_2 & 0 \end{pmatrix}. \quad (11)$$

The mass term is invariant under the orbifold twist (8) provided

$$\{\mathcal{B}, \mathcal{M}\} = 0. \quad (12)$$

### D. Consistency conditions

The periodicity and reflection transformations are not independent since  $-y = [-(y+L)] + L$  and  $-(-y) = y$ . These imply, respectively,

$$\mathcal{B} = \mathcal{A} \mathcal{B} \mathcal{A}, \quad (13)$$

$$\mathcal{B}^2 = 1, \quad (14)$$

for the fermions. For the  $Pi - Rj$  BC ( $i, j = 1, 2$ ) the corresponding constraints on the gauge bosons give (no sum over  $i$  and  $j$ )

$$[\tau_a, \tilde{\mathcal{V}}_j \mathcal{V}_i \tilde{\mathcal{V}}_j \mathcal{V}_i^\dagger] = 0, \quad (15)$$

$$[\tau_a, \tilde{\mathcal{V}}_i^2] = 0, \quad (16)$$

where  $\mathcal{V}_1 = \mathcal{U}_1$ ,  $\tilde{\mathcal{V}}_1 = \tilde{\mathcal{U}}_1$  and  $\mathcal{V}_2 = \mathcal{U}_2^*$ ,  $\tilde{\mathcal{V}}_2 = \tilde{\mathcal{U}}_2^*$ .

These conditions imply that  $\tilde{\mathcal{V}}_j \mathcal{V}_i \tilde{\mathcal{V}}_j \mathcal{V}_i^\dagger$  and  $\tilde{\mathcal{V}}_i^2$  belong to the center of the group. If the representation generated by  $\{\tau_a\}$  is split into its irreducible components, the projection of these matrices onto each irreducible subspace must be proportional to the unit matrix as a consequence of the Schur's lemma. We now examine this and other similar restrictions imposed by the local symmetry.

### E. Gauge invariance

Under a gauge transformation  $\Omega$  the fields transform as

$$\begin{aligned} A_N &\rightarrow A'_N = \frac{1}{ig_5} \Omega D_N \Omega^\dagger \quad \text{and} \\ \chi &\rightarrow \chi' = \begin{pmatrix} \Omega^* & 0 \\ 0 & \Omega \end{pmatrix} \chi \equiv \mathcal{O}^* \chi. \end{aligned} \quad (17)$$

For the theory to be gauge invariant the gauge-transformed fields should satisfy the same boundary conditions<sup>5</sup> (2) and (8):

$$\begin{aligned} \chi'(y+L) &= \mathcal{A}^* \chi'(y), \\ \chi'(-y) &= \gamma_5 \mathcal{B}^* \chi'(y), \end{aligned} \quad (18)$$

$$\begin{aligned} A'_N(y+L) &= \begin{cases} +U_1^\dagger A'_N(y) U_1 & (P1), \\ -U_2^\dagger A'_N(y) U_2 & (P2), \end{cases} \\ A'_N(-y) &= \begin{cases} (-1)^{s_N} \tilde{U}_1^\dagger A'_N(y) \tilde{U}_1 & (R1), \\ (-1)^{1-s_N} \tilde{U}_2^\dagger A'_N(y) \tilde{U}_2 & (R2). \end{cases} \end{aligned} \quad (19)$$

We consider first the constraints implied by imposing  $P1$ . Using the transformation properties of  $\chi$  we find that this choice of BC respects gauge invariance provided

$$\mathcal{O}(y+L) = \mathcal{A} \mathcal{O}(y) \mathcal{A}^\dagger \quad (P1). \quad (20)$$

Similarly, the transformation properties of the gauge fields require

$$(\Omega D_N \Omega^\dagger)_{y+L} = (U_1^\dagger \Omega D_N \Omega^\dagger U_1)_y, \quad (21)$$

which leads to

$$(\Omega \partial_N \Omega^\dagger)_{y+L} = (U_1^\dagger \Omega (\partial_N \Omega^\dagger) U_1)_y, \quad (22)$$

$$[T_a, \Omega^\dagger(y) U_1 \Omega(y+L) U_1^\dagger] = 0,$$

where we used (2) to express  $A_N(y+L)$  in terms of  $A_N(y)$ . In terms of  $\mathcal{O}$  these constraints become

$$\begin{aligned} (\mathcal{O} \partial_N \mathcal{O}^\dagger)_{y+L} &= (U_1^\dagger \mathcal{O} (\partial_N \mathcal{O}^\dagger) U_1)_y, \\ [\tau_a, \mathcal{O}^\dagger(y) U_1 \mathcal{O}(y+L) U_1^\dagger] &= 0. \end{aligned} \quad (23)$$

Using then (20) we find

$$[\mathcal{O} \partial_N \mathcal{O}^\dagger, U_1 \mathcal{A}] = 0, \quad [\tau_a, \mathcal{O}^\dagger U_1 \mathcal{A} \mathcal{O} \mathcal{A}^\dagger U_1^\dagger] = 0, \quad (24)$$

where  $\mathcal{O}$  is evaluated at  $y$ .

For connected gauge groups one can always write  $\mathcal{O}(y) = \exp(i\omega_a(y)\tau_a)$ ; in this case the first equation in (24) is satisfied once (5) is imposed. The second equation in (24) is also satisfied since by (5)  $U_1 \mathcal{A}$  commutes with

<sup>5</sup>Note that the gauge invariance defined as a gauge transformation preserving the Lagrangian and the BC corresponds to “the residual gauge invariance” in the language used by Hosotani in the fourth paper of Ref. [3].

all the  $\mathcal{O}$ . So, the bosonic BC are gauge invariant as a consequence of the symmetry of the Lagrangian under the twist operation (2) and of the gauge symmetry of the fermionic BC (18).

Similar arguments for the other three types of boundary conditions show that for any choice  $Pi - Rj$  the theory retains its local symmetry provided (5) and (10) are valid and if the gauge transformations are restricted by the conditions

$$\mathcal{O}(y+L) = \mathcal{A} \mathcal{O}(y) \mathcal{A}^\dagger \quad \text{and} \quad \mathcal{O}(-y) = \mathcal{B} \mathcal{O}(y) \mathcal{B}^\dagger. \quad (25)$$

For non-Abelian groups it is not too difficult (at least for infinitesimal transformations) to show that the converse, i.e. that the gauge invariance of the bosonic BC (19) implies that the invariance of the fermionic ones (18) [which is equivalent to (25)] also holds, provided (5) and (10) are satisfied. In other words, the bosonic BC are gauge invariant if and only if the fermionic BC are gauge invariant, provided the theory is symmetric under the twist operations (5) and (10). For Abelian groups a similar calculation leaves a phase ambiguity.

When the fields are expanded in Fourier series, conditions (5) and (10) often forbid the presence of zero modes for some of  $A_N^a$ . The absence of certain gauge-boson zero modes is directly related to constraints which must be satisfied by the gauge functions  $\omega_a(y)$  to obey (25).

For instance, as a prelude to the discussion of various Abelian examples in Sec. III A, it is worth listing here for a  $U(1)$  gauge theory the forbidden gauge-boson modes together with the restrictions on the allowed gauge transformation that follow from (25):

- (i)  $P1/P2$ : The gauge invariance of BC requires periodicity ( $P1$ ) or antiperiodicity ( $P2$ );  $\Lambda(y+L) = \pm \Lambda(y)$  [ $\Lambda(y)$  is the  $U(1)$  gauge function:  $A_M \rightarrow A_M + \partial_M \Lambda$ ]. Note that for  $P2$  the antiperiodicity of  $A_\mu(y)$  eliminates a massless photon for this choice of BC.
- (ii)  $R1/R2$ : Here for the invariance of the BC one needs  $\Lambda(-y) = \pm \Lambda(y)$ . In particular a massless gauge-boson mode is not allowed by the odd boundary condition  $R2$ .

Note that  $y$ -independent gauge transformations are not allowed for  $P2$  or  $R2$  due, respectively, to the antiperiodicity or asymmetry of  $\Lambda(y)$ ; in these cases the gauge symmetry of the zero-mode sector (i.e. KK modes of  $y$ -independent 5D fields) is broken completely. This will be discussed in detail in Sec. V B.

Though the BC may reduce the gauge symmetry within the zero-mode sector, *the whole theory remains 5D gauge invariant*. It is not difficult to show that, at least for infinitesimal gauge transformations, there exists a basis (in general different basis must be adopted for the periodicity and the orbifold conditions) such that (25) reduces to  $\omega_a(y+L) = \pm \omega_a(y)$  and  $\omega_a(-y) = \pm \omega_a(y)$  (signs are

uncorrelated). Therefore, choosing appropriate values for  $\omega(0)$  and  $\omega(\pm L/2)$  it is always possible to find *all* nonzero, continuous and differentiable  $\omega_a(y)$  such that (25) is satisfied. The initial symmetry group remains unchanged since *all*  $\omega_a(y)$  are nonzero, though their functional form is constrained by the above periodicity and reflection conditions. For a similar discussion see also [10].

For example, consider an  $SU(2)$  theory with a single doublet and  $(P1 - R1)$  BC. Taking  $\Gamma = U_1 = i\sigma_3$ ,  $\tilde{\Gamma} = -i\tilde{U}_1 = \sigma_1$  and  $Y = \tilde{Y} = 0$  (so  $\mathcal{A}, \mathcal{B} \neq \mathbb{1}$ ) the conditions, (25), on the gauge transformation functions  $\Omega = \exp(i\sigma^a \omega_a)$  imply

$$\begin{aligned} \omega_1(y) &= -\omega_1(y+L) = +\omega_1(-y), \\ \omega_2(y) &= -\omega_2(y+L) - \omega_2(-y), \\ \omega_3(y) &= +\omega_3(y+L) = -\omega_3(-y). \end{aligned} \quad (26)$$

Therefore the theory (including the BC) will have a local  $SU(2)$  symmetry provided the  $\omega_a(y)$  satisfy the above constraints. If we had chosen instead  $\Gamma = U_1 = \tilde{\Gamma} = \tilde{U}_1 = \mathbb{1}$ ,  $Y = \tilde{Y} = 0$  ( $\mathcal{A} = \mathcal{B} = \mathbb{1}$ ) then the BC are gauge invariant provided  $\omega_a(y) = \omega_a(y+L) = \omega_a(-y)$  ( $a = 1, 2, 3$ ); since the  $\omega_a$  are all nonzero, this is again a local  $SU(2)$  theory, but not with the same local group as in the first case, in fact, the only common element is  $\Omega = \mathbb{1}$ . This also illustrates another interesting fact, namely, that nontrivial choices of  $\mathcal{A}$  and  $\mathcal{B}$ , i.e.  $\mathcal{A} \neq \mathbb{1}$  and  $\mathcal{B} \neq \mathbb{1}$ , do not reduce the 5D local symmetry group (as we have just argued the group remains the same), but it may simply change it as we have observed in the above example.

Let us briefly discuss the gauge symmetry of the zero-mode sector in the above example (26). For  $y$ -independent transformations the periodicity condition  $P1$  requires  $\omega_{1,2} = 0$ , while  $R1$  requires  $\omega_3 = 0$ . In this case the gauge group of the light sector is completely broken.

The above scheme of gauge symmetry breaking in the zero-mode sector by BC (the Scherk-Schwarz mechanism) could be also viewed from the following perspective. The 5D gauge symmetry is associated with a set of unconstrained gauge functions  $\omega_a(y)$ . Imposing BC restricts the set of allowed  $\omega_a(y)$ 's, for instance requiring them to be antiperiodic and even. Therefore the symmetry is ‘‘reduced’’ by which we mean that none of the generators is broken (none of the  $\omega_a$  is required to vanish identically by the BC) and yet *the zero-mode sector has only a subgroup of the original group*. For instance, in a  $U(1)$  gauge model with  $R2$ ,  $A_\mu(y)$  has no zero mode.

### F. General solutions for the allowed boundary conditions

The conditions (5) and (10) significantly constrain the form of  $\mathcal{A}$  and  $\mathcal{B}$ . To derive the general structure of these matrices we decompose  $\Psi$  in terms of multiplets  $\psi_r$  being each in an irreducible representation  $r$  of the gauge group.

As a preliminary result we first show that when  $r$  is complex we can assume without loss of generality that  $\psi$  contains no multiplet transforming according to the complex-conjugate irreducible representation  $\bar{r}$ .

To see this first note that given the structure of the Lagrangian we can assume that the mass matrix is diagonal, and we will denote by  $m_r$  the eigenvalue associated with  $\psi_r$ . Then if the theory does originally contains a fermion multiplet  $\psi_{\bar{r}}$  transforming according to the irreducible representation  $\bar{r}$ , the terms in  $\mathcal{L}$  where this field appears are

$$\mathcal{L} \bar{r} = \bar{\psi}_{\bar{r}} [i\gamma^N (\partial_N + ig_5 T_a \bar{r} A_N^a) - m_{\bar{r}}] \psi_{\bar{r}}, \quad (27)$$

where the  $T_a^{(\bar{r})}$  generate the corresponding representation. It is then possible to define a field  $\psi'_r = (\psi_{\bar{r}})^c$  (that transforms according to the complex-conjugate irreducible representation  $r$ ) in terms of which

$$\mathcal{L} \bar{r} = \bar{\psi}'_r [i\gamma^N (\partial_N + ig_5 T_a r A_N^a) - m'_r] \psi'_r, \quad (28)$$

where  $m'_r = -m_{\bar{r}}$  and  $T_a^{(r)} = -(T_a^{(\bar{r})})^*$ . Since we can replace each  $\psi_{\bar{r}}$  by its corresponding  $\psi'_r$ , we can assume that  $\Psi$  contains no multiplets in the complex-conjugate irreducible representation  $\bar{r}$ .

This way of eliminating conjugate representations does not lead to any simplifications for real or pseudoreal representations  $r_u$  since the corresponding generators satisfy

$$T_a^{(\bar{r}_u)} = [-T_a^{(r_u)}]^* = S_u T_a^{(r_u)} S_u^\dagger, \quad (29)$$

for some unitary matrix  $S_u$  that is (anti)symmetric for (pseudo)real representations.

The above arguments imply that we can choose fields such that

$$T_a = \text{diag}(\dots, \mathbb{1}_{n_\ell} \otimes T_a^{(r_\ell)}, \dots, \mathbb{1}_{n_u} \otimes T_a^{(r_u)}, \dots), \quad (30)$$

where we assume the theory contains  $n_\ell$  flavors in the complex irreducible representation  $r_\ell$  and  $n_u$  flavors in the (pseudo)real irreducible representation  $r_u$ . In this expression as in the rest of the paper a matrix of the form  $\mathcal{F} \otimes \mathcal{G}$  is understood as having  $\mathcal{F}$  ( $\mathcal{G}$ ) act on the flavor (gauge) indices, and  $\mathbb{1}_n$  denotes the  $n \times n$  unit matrix.

Letting  $d_{\ell,u}$  be the dimension of  $r_{\ell,u}$  we define

$$\begin{aligned} F &= \text{diag}(\dots, \mathbb{1}_{n_\ell} \otimes \mathbb{1}_{d_\ell}, \dots, \mathbb{1}_{n_u} \otimes \mathbb{1}_{d_u}, \dots; \dots, \mathbb{1}_{n_\ell} \\ &\otimes \mathbb{1}_{d_\ell}, \dots, \mathbb{1}_{n_u} \otimes S_u, \dots), \end{aligned} \quad (31)$$

so that  $\tau_a = F \tau'_a F^\dagger$ , where

$$\begin{aligned} \tau'_a &= \text{diag}(\dots, \mathbb{1}_{n_\ell} \otimes T_a^{(r_\ell)}, \dots, \mathbb{1}_{n_u} \otimes T_a^{(r_u)}, \dots; \dots, \mathbb{1}_{n_\ell} \\ &\otimes T_a^{(\bar{r}_\ell)}, \dots, \mathbb{1} \otimes T_a r_u, \dots). \end{aligned} \quad (32)$$

Adopting the Schur's lemma and the grand orthogonality theorem [used to eliminate the possibility that the  $T_a^{(r)}$  might be linearly dependent] the twist-invariance conditions  $[\tau'_a, F^\dagger \mathcal{U}_i \mathcal{A} F] = 0$ ,  $[\tau'_a, F^\dagger \tilde{\mathcal{U}}_i \mathcal{B} F] = 0$ , imply that

$F^\dagger \mathcal{U}_i \mathcal{A} F$  and  $F^\dagger \tilde{\mathcal{U}}_i \mathcal{B} F$  have no entries connecting two inequivalent representations, and that entries connecting equivalent representations will be diagonal in the gauge indices. Explicitly we obtain

$$F^\dagger \mathcal{U}_i \mathcal{A} F = \begin{pmatrix} X_\ell \otimes \mathbb{1}_{d_\ell} & 0 & 0 & 0 \\ 0 & X_u \otimes \mathbb{1}_{d_u} & 0 & Y'_u \otimes \mathbb{1}_{d_u} \\ 0 & 0 & X'_\ell \otimes \mathbb{1}_{d_\ell} & 0 \\ 0 & Y_u \otimes \mathbb{1}_{d_u} & 0 & X'_u \otimes \mathbb{1}_{d_u} \end{pmatrix},$$

$$F^\dagger \tilde{\mathcal{U}}_i \mathcal{B} F = \begin{pmatrix} \tilde{X}_\ell \otimes \mathbb{1}_{d_\ell} & 0 & 0 & 0 \\ 0 & \tilde{X}_u \otimes \mathbb{1}_{d_u} & 0 & \tilde{Y}'_u \otimes \mathbb{1}_{d_u} \\ 0 & 0 & \tilde{X}'_\ell \otimes \mathbb{1}_{d_\ell} & 0 \\ 0 & \tilde{Y}_u \otimes \mathbb{1}_{d_u} & 0 & \tilde{X}'_u \otimes \mathbb{1}_{d_u} \end{pmatrix}. \quad (33)$$

If  $U_i = \exp\{iu_a^i T_a\}$ , we denote by  $U_{i;\ell} = \exp\{iu_a^i T_{a r \ell}\}$ ,  $i = 1, 2$  and similarly for  $U_{i;u}$ ,  $\tilde{U}_{i;\ell}$  and  $\tilde{U}_{i;u}$ . Then, using the unitarity of  $\mathcal{U}_i$  and  $F$  we find

$$P1 : \Gamma = \text{diag}(\cdots, X_{1;\ell} \otimes U_{1;\ell}^\dagger, \cdots, X_{1;u} \otimes U_{1;u}^\dagger, \cdots),$$

$$Y = \text{diag}(\cdots, 0, \cdots, Y_{1;u} \otimes U_{1;u}^T S_u, \cdots),$$

$$P2 : \Gamma = \text{diag}(\cdots, 0, \cdots, Y_{2;u} \otimes U_{2;u}^\dagger S_u, \cdots),$$

$$Y = \text{diag}(\cdots, X_{2;\ell} \otimes U_{2;\ell}^T, \cdots, X_{2;u} \otimes U_{2;u}^T, \cdots),$$

$$R1 : \tilde{\Gamma} = -\text{diag}(\cdots, \tilde{X}_{1;\ell} \otimes \tilde{U}_{1;\ell}^\dagger, \cdots, \tilde{X}_{1;u} \otimes \tilde{U}_{1;u}^\dagger, \cdots),$$

$$\tilde{Y} = \text{diag}(\cdots, 0, \cdots, \tilde{Y}_{1;u} \otimes \tilde{U}_{1;u}^T S_u, \cdots),$$

$$R2 : \tilde{\Gamma} = -\text{diag}(\cdots, 0, \cdots, \tilde{Y}_{2;u} \otimes \tilde{U}_{2;u}^\dagger S_u, \cdots),$$

$$\tilde{Y} = \text{diag}(\cdots, \tilde{X}_{2;\ell} \otimes \tilde{U}_{2;\ell}^T, \cdots, \tilde{X}_{2;u} \otimes \tilde{U}_{2;u}^T, \cdots). \quad (34)$$

The specific form of  $\mathcal{A}$  and  $\mathcal{B}$  in (3) and (9) allows  $X'_u, Y'_u, \tilde{X}'_u, \tilde{Y}'_u$  to be written in terms of  $X_u, Y_u, \tilde{X}_u, \tilde{Y}_u$ , but these relations will not be displayed as they are not needed.

The unitarity of  $\mathcal{A}$  and  $\mathcal{B}$  implies

$$X_{i;\ell}^\dagger X_{i;\ell} = \mathbb{1}_{n_\ell}, \quad \tilde{X}_{i;\ell}^\dagger \tilde{X}_{i;\ell} = \mathbb{1}_{n_\ell},$$

$$X_{i;u}^\dagger X_{i;u} + Y_{i;u}^\dagger Y_{i;u} = \mathbb{1}_{n_u}, \quad \tilde{X}_{i;u}^\dagger \tilde{X}_{i;u} + \tilde{Y}_{i;u}^\dagger \tilde{Y}_{i;u} = \mathbb{1}_{n_u},$$

$$X_{i;u}^T Y_{i;u} = \pm Y_{i;u}^T X_{i;u}, \quad \tilde{X}_{i;u}^T \tilde{Y}_{i;u} = \pm \tilde{Y}_{i;u}^T \tilde{X}_{i;u}, \quad (35)$$

where the upper (lower) signs correspond to (pseudo)real irreducible representations.

The consistency condition  $\mathcal{B} = \mathcal{B}^\dagger$  requires, for complex representations,

$$R1 : \tilde{X}_{1;\ell} = \tilde{c}_\ell \tilde{X}_{1;\ell}^\dagger, \quad \tilde{U}_{1;\ell}^2 = \tilde{c}_\ell \mathbb{1}_{d_\ell}, \quad |\tilde{c}_\ell|^2 = 1, \quad (36)$$

$$R2 : \tilde{X}_{2;\ell} = \tilde{c}_\ell \tilde{X}_{2;\ell}^\dagger, \quad \tilde{U}_{2;\ell} \tilde{U}_{2;\ell}^* = \tilde{c}_\ell \mathbb{1}_{d_\ell}, \quad \tilde{c}_\ell^2 = 1,$$

while for real or pseudoreal representations we find

$$R1 : \tilde{X}_{1;u} = \tilde{c}_u \tilde{X}_{1;u}^\dagger, \quad \tilde{Y}_{1;u} = \pm \tilde{c}_u \tilde{Y}_{1;u}^\dagger, \quad \tilde{U}_{1;u}^2 = \tilde{c}_u \mathbb{1}_{d_u}, \quad \tilde{c}_u^2 = 1,$$

$$R2 : \tilde{Y}_{2;u} = \tilde{c}_u \tilde{Y}_{2;u}^\dagger, \quad \tilde{X}_{2;u} = \tilde{c}_u \tilde{X}_{2;u}^\dagger, \quad \tilde{U}_{2;u} \tilde{U}_{2;u}^* = \tilde{c}_u \mathbb{1}_{d_u}, \quad \tilde{c}_u^2 = 1, \quad (37)$$

where the (lower) upper sign refers to a (pseudo)real representation. For  $R2$  we used the fact that we can assume  $S_u^2 = \mathbb{1}$ .<sup>6</sup> Notice that the above constraints on the matrices  $U_{i;r}$  are sufficient to obey the gauge-boson-consistency constraints (16).

The constraints required by  $\mathcal{A}\mathcal{B} = (\mathcal{A}\mathcal{B})^\dagger$  can be obtained in a similar way. Using Table I we define the matrices  $K$  and  $L$ . In order to fulfill the condition  $\mathcal{A}\mathcal{B} = (\mathcal{A}\mathcal{B})^\dagger$  these matrices should satisfy

$$K_{ij}^{(r)} = \lambda_{ij}^{(r)} K_{ij}^{(r)\dagger}, \quad L_{ij}^{(r)} = s_{ij}^{(r)} L_{ij}^{(r)T}; \quad (s_{ij}^{(r)})^2 = 1 \quad (38)$$

(no sum over  $i, j = 1, 2$ ). For complex representations  $|\lambda_{ij}^{(r)}| = 1$  while for noncomplex representations

$$\lambda_{11}^{(u)} = \pm s_{11}^{(u)}, \quad \lambda_{12}^{(u)} = s_{12}^{(u)}, \quad (39)$$

$$\lambda_{22}^{(u)} = \pm s_{22}^{(u)}, \quad \lambda_{21}^{(u)} = s_{21}^{(u)},$$

where the upper (lower) sign refers to a (pseudo)real representation. The corresponding restrictions on the matrices  $U_{i;r}$  are given in Table II

It is worth noting that the consistency conditions (15) also lead to constraints of the form given in Table II, but with  $\lambda_{ij}^{(r)}, s_{ij}^{(r)}$  arbitrary complex numbers; the additional restrictions (38) and (39) follow exclusively from the Hermiticity of  $\mathcal{A}\mathcal{B}$ .

The expressions (34)–(37) and Table II together with  $|\lambda_{ij}^{(r)}| = 1$  and (39) give the most general form for the matrices  $\mathcal{A}$ ,  $\mathcal{B}$ ,  $\mathcal{U}_i$  and  $\tilde{\mathcal{U}}_j$ . In particular

- (i) The matrices  $\Gamma, Y, \tilde{\Gamma}$  and  $\tilde{Y}$  do not mix  $\psi_r$  and  $\psi_s$  unless  $r$  is equivalent to  $s$  or  $\bar{s}$ .
- (ii) For the BC  $P1$  and  $R1$  ( $P2$  and  $R2$ ), in the subspace spanned by all multiplets in the same *complex* irreducible representation  $r$ , the matrices  $Y$  and  $\tilde{Y}$  ( $\Gamma$  and  $\tilde{\Gamma}$ ) vanish. In contrast,  $\Gamma$  and  $\tilde{\Gamma}$  ( $Y$  and  $\tilde{Y}$ ) are direct products of unitary rotation in flavor indices and global gauge transformation in gauge indices.
- (iii) In the subspace spanned by all multiplets carrying the same (*pseudo*) *real* irreducible representation  $r$  in general  $Y$  ( $\tilde{Y}$ ) and  $\Gamma$  ( $\tilde{\Gamma}$ ) are nonzero.

One of the virtues of including the generalized twist operations is that they allow *all* mixing consistent with gauge invariance; a more restricted standard set ( $Y = \tilde{Y} = 0$ ) of BC would not, for example, allow a mixing between  $\psi_r$  and  $\psi_r^c$  even though they might transform in the same way under the local symmetry group. The price we pay for this generalization is the breaking by the BC of global

<sup>6</sup>For a noncomplex representation (dropping the  $u$  subscript) and taking a basis where  $C_i$  are the Cartan generators and  $E_\alpha$  the root generators, the conjugate representation is generated by  $C_i = S C_i S^\dagger = -C_i$ ,  $E'_\alpha = S E_\alpha S^\dagger = -E_{-\alpha}$  from which it follows that  $S^2$  commutes with all the generators and so  $S^2 = \sigma \mathbb{1}$  for some complex number  $\sigma$ ,  $|\sigma| = 1$ . Redefining  $S \rightarrow S/\sqrt{\sigma}$  shows we can take  $S^2 = \mathbb{1}$ .

TABLE I. Definition of the matrices  $K$  and  $L$ ; the upper (lower) signs refer to (pseudo)real representations

BC	Noncomplex		Complex
$P1 - R1$	$K_{11}^{(u)} = -X_{1;u}\tilde{X}_{1;u} \pm Y_{1;u}^* \tilde{Y}_{1;u}$	$L_{11}^{(u)} = X_{1;u}^* \tilde{Y}_{1;u} + Y_{1;u} \tilde{X}_{1;u}$	$K_{11}^{(\ell)} = -X_{1;\ell}\tilde{X}_{1;\ell}$
$P1 - R2$	$K_{12}^{(u)} = -X_{1;u}\tilde{Y}_{2;u} \pm Y_{1;u}^* \tilde{X}_{2;u}$	$L_{12}^{(u)} = X_{1;u}^* \tilde{X}_{2;u} + Y_{1;u} \tilde{Y}_{2;u}$	$L_{12}^{(\ell)} = X_{1;\ell}^* \tilde{X}_{2;\ell}$
$P2 - R1$	$K_{21}^{(u)} = -Y_{2;u}\tilde{X}_{1;u} + X_{2;u}^* \tilde{Y}_{1;u}$	$L_{21}^{(u)} = \pm Y_{2;u}^* \tilde{Y}_{1;u} + X_{2;u} \tilde{X}_{1;u}$	$L_{21}^{(\ell)} = X_{2;\ell} \tilde{X}_{1;\ell}$
$P2 - R2$	$K_{22}^{(u)} = -Y_{2;u}\tilde{Y}_{2;u} + X_{2;u}^* \tilde{X}_{2;u}$	$L_{22}^{(u)} = \pm Y_{2;u}^* \tilde{X}_{2;u} + X_{2;u} \tilde{Y}_{2;u}$	$K_{22}^{(\ell)} = X_{2;\ell}^* \tilde{X}_{2;\ell}$

fermion number (for noncomplex representations), and possibly other global symmetries.

There is a comment here in order. The twist-invariance conditions, (5) and (10) guarantee that the Lagrangian is symmetric under the twist operations defined by (2) and (8). In addition the fermionic and bosonic twist operations must satisfy the consistency conditions, (13) and (14) and (15) and (16), respectively. It is interesting to observe that our general solutions (37) and Table II show that in fact the fermionic consistency conditions (13) and (14) *imply* that the bosonic ones (15) and (16) are satisfied. This remarkable fact has been confirmed in all the examples considered in Secs. III and IV; the solutions for  $\mathcal{U}_i$  obtained by imposing the fermionic consistency condition automatically satisfy the bosonic ones.

### G. Vacuum expectation values

One property exhibited by many 5D systems is the possibility that  $A_4$  may acquire a vacuum expectation value, which can lead to a variety of interesting consequences such as spontaneous breaking of  $CP$  [7]. In order to determine the constraints imposed on such a vacuum expectation value by the various boundary conditions described above we define

$$\mathbb{A} \equiv \begin{pmatrix} \langle A_4 \rangle & 0 \\ 0 & -\langle A_4 \rangle^* \end{pmatrix}, \quad (40)$$

which is preserved by  $Pi - Rj$  provided

$$[\mathbb{A}, \mathcal{U}_i] = 0, \quad \{\mathbb{A}, \tilde{\mathcal{U}}_j\} = 0. \quad (41)$$

For a non-Abelian group there are always nontrivial solutions to these equations. For an Abelian groups, however, only the case  $P1 - R2$  allows a nonzero vacuum expectation value. Note also that even if a nonzero vacuum expectation value is allowed this does not imply that such a  $\langle A_4 \rangle$  will correspond to absolute minima of the effective potential; this can be only decided by explicitly calculating the

 TABLE II. Constraints on the matrices  $U$ .

$P1 - R1$	$\tilde{U}_{1;r} U_{1;r} = \lambda_{11}^{(r)} U_{1;r}^\dagger \tilde{U}_{1;r}^\dagger$
$P1 - R2$	$\tilde{U}_{2;r} U_{1;r} = s_{12}^{(r)} U_{1;r}^\dagger \tilde{U}_{2;r}^\dagger$
$P2 - R1$	$\tilde{U}_{1;r}^* U_{2;r} = s_{21}^{(r)} U_{2;r}^\dagger \tilde{U}_{1;r}^\dagger$
$P2 - R2$	$\tilde{U}_{2;u}^* U_{2;r} = \lambda_{22}^{(r)} U_{2;r}^\dagger \tilde{U}_{2;r}^\dagger$

effective potential and will depend on the fermion content of the theory.

### H. $C$ , $P$ and $CP$

In 5D the parity transformation acting on the space-time points is defined as follows:  $x^{0,4} \rightarrow x^{0,4}$  and  $x^i \rightarrow -x^i$ , for  $i = 1, 2, 3$ . Therefore for the parity acting on fermionic fields and for the charge conjugation we obtain:

$$\chi \xrightarrow{P} \gamma_0 \gamma_4 \chi, \quad \chi \xrightarrow{C} \chi^c = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \chi. \quad (42)$$

Then under  $CP$  we obtain

$$\chi \xrightarrow{CP} \gamma_0 \gamma_4 \mathcal{D} \chi \equiv \gamma_0 \gamma_4 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \chi, \quad (43)$$

while the gauge fields transform as

$$A_i \xrightarrow{CP} + A_i^T, \quad A_{0,4} \xrightarrow{CP} - A_{0,4}^T, \quad (44)$$

where  $i = 1, 2, 3$ .

One can generalize these definitions by noting that the kinetic term in  $\mathcal{L}$  is invariant under unitary flavor mixing [11] among fields belonging to the same representation, so in (43) we can replace

$$\mathcal{D} = \begin{pmatrix} 0 & -\Theta^* \\ \Theta & 0 \end{pmatrix} \quad \text{with } \Theta^\dagger \Theta = 1. \quad (45)$$

In that general case we find

$$A_i \xrightarrow{CP} + \Theta A_i^T \Theta^\dagger, \quad A_{0,4} \xrightarrow{CP} - \Theta A_{0,4}^T \Theta^\dagger, \quad (46)$$

where  $i = 1, 2, 3$ .

The condition for the invariance of the mass term under  $CP$  is  $\{\mathcal{M}, \mathcal{D}\} = 0$ , or, equivalently,  $M\Theta^* = \Theta^* M^*$ . Since  $M$  is Hermitian, we can always adopt a basis where it is real and diagonal, in which case this condition reduces to  $[M, \Theta] = 0$ . It follows that in the absence of  $CP$  violation (CPV) we can find a basis where both  $M$  and  $\Theta$  are diagonal; one can then choose the field phases such that the matrix  $\mathcal{D}$  is given by the simple expression used in (43). If, on the other hand  $\Theta$  is such that (in a basis where  $M$  is real and diagonal)  $[M, \Theta] \neq 0$ , then the mass term will explicitly break  $CP$ .

The boundary conditions will preserve  $CP$  invariance only if

$$\begin{aligned} [\mathcal{A}^*, \mathcal{D}] &= 0, & U_i &= U_i^* \quad (i = 1, 2), \\ \{\mathcal{B}^*, \mathcal{D}\} &= 0, & \tilde{U}_i &= \tilde{U}_i^* \quad (i = 1, 2), \end{aligned} \quad (47)$$

or, equivalently,

$$\begin{aligned} \Theta^\dagger \Gamma \Theta &= \Gamma^*, & \Theta^\dagger \tilde{\Gamma} \Theta &= \tilde{\Gamma}^*, \\ \Theta^T \Upsilon \Theta &= \Upsilon^*, & \Theta^T \tilde{\Upsilon} \Theta &= \tilde{\Upsilon}^*, \end{aligned} \quad (48)$$

which, for  $\Theta = \mathbb{1}$ , merely requires  $\mathcal{A}$  and  $\mathcal{B}$  to be real. If any one of these conditions is violated the boundary conditions will break  $CP$  explicitly.

This theory also contains a third source of CPV: the vacuum expectation value of  $A_4$ . If  $\langle A_4 \rangle \neq 0$  then we can take this matrix as proportional to a Cartan generator<sup>7</sup> which is a symmetric matrix; then

$$A_4 \xrightarrow{CP} -A_4, \quad (49)$$

so that such a vacuum expectation value violates  $CP$  spontaneously.

Summarizing: the theory described by (1) will respect  $CP$  only if  $[M, \Theta] = \langle A_4 \rangle = 0$  and if the conditions (47) are obeyed.

The simplest illustration of  $CP$  violation in the context of 5D models has been considered in [7]. It was shown there that if at least two fermions are present, then for a compactification on a circle a nonzero  $\langle A_4 \rangle$  appears at the one-loop level, so that  $CP$  could be broken spontaneously. It turns out that in 4D theory, after a KK decomposition, in a unitary gauge only the zero mode of  $A_4$  remains with  $CP$  violating coupling of the form  $A_4(x)\psi_n(x)(a + ib\gamma_5)\psi(x)$ , where  $a, b$  are real numbers and  $\psi_n(x)$  is the  $n$ th fermionic KK mode. As shown in [7], an interaction of this form can, for instance, lead at the one-loop level<sup>8</sup> to nonzero electric dipole moment of a fermion. An analogous example for the orbifold compactification is discussed in the appendix.

### III. ABELIAN EXAMPLES

In this section we will illustrate the consequences of the above generalized boundary conditions for the case of an Abelian group. We first study the case of a single fermion and then that of two fermions that exhibit some new features.

#### A. One fermion

For a single fermion of mass  $m$  and charge  $q$  (in units of  $g_5$ ) we have  $\mathcal{M} = m\sigma_3$  and  $\tau = q\sigma_3$  (there is a single group generator so we drop the subindex  $a$ ). Imposing the previous constraints on  $\mathcal{A}$  and  $\mathcal{B}$  and using the freedom to

<sup>7</sup>That is, there is a group rotation that takes this matrix into a Cartan generator times a real number

<sup>8</sup>As the vacuum expectation value of  $A_4$  is generated at the one-loop, therefore in fact, the electric dipole moment emerges at the two-loop level.

TABLE III. Matrices  $\mathcal{A}, \mathcal{B}$  for the Abelian models with one fermion;  $u^2 + v^2 = 1$  and  $s_{a,b}^2 = 1$  (the signs  $s_a$  and  $s_b$  are uncorrelated).

	$P1 - R1$	$P1 - R2$	$P2 - R1$	$P2 - R2$
$\mathcal{A}$	$s_a \mathbf{1}$	$u \mathbf{1} + iv \sigma_3$	$-i \sigma_2$	$-i \sigma_2$
$\mathcal{B}$	$-s_b \sigma_3$	$\sigma_1$	$-s_b \sigma_3$	$s_b \sigma_1$

choose the global phase of the fields to eliminate some of the phases, we find the expressions in Table III. The bare-mass term in  $\mathcal{L}$  and a possible nonzero vacuum expectation value  $\langle A_4 \rangle$  are allowed only by the combination  $P1 - R2$ ; in this case the mass term will conserve  $CP$ .

Whenever BC involving  $P2$  are chosen the fermion field obeys the periodicity condition  $\Psi(y + L) = \Psi^c(y)$ , which leads to  $\Psi(y + 2L) = -\Psi(y)$ . Then

$$\begin{aligned} P2: \Psi(y) &= \frac{1}{\sqrt{2L}} \sum_{n=-\infty}^{\infty} e^{i(n+1/2)\pi y/L} \psi_n, \\ \psi_n &= e^{-i(n+1/2)\pi} \psi_{-n-1}^c. \end{aligned} \quad (50)$$

If we also impose  $R1$  this expression is further constrained by  $\Psi(-y) = s_b \gamma_5 \Psi(y)$ , as a result we find

$$\begin{aligned} \psi_n &= \begin{pmatrix} s_b (-1)^n \sigma_2 \varphi_n^* \\ \varphi_n \end{pmatrix}, \\ \varphi_{-n-1} &= (-1)^n \sigma_2 \varphi_n^* \quad (P2 - R1), \end{aligned} \quad (51)$$

where  $\varphi_n$  is a 2-component spinor. For these boundary conditions ( $P2 - R1$ ) a bare-mass term for the fermion is not allowed in the Lagrangian, nonetheless the  $\varphi$  receive a mass of order  $1/L$  from the kinetic terms:

$$\begin{aligned} \int_0^L dy \bar{\Psi} \gamma^4 i \partial_4 \Psi &= \sum_{n=0}^{\infty} \frac{i s_b (-1)^n \pi (2n+1)}{2L} \varphi_n^T \sigma_2 \varphi_n \\ &+ \text{H.c.} \quad (P2 - R1). \end{aligned} \quad (52)$$

Similar results are obtained for  $P2 - R2$ :

$$\begin{aligned} \psi_n &= \begin{pmatrix} -i s_b \sigma_2 \varphi_n^* \\ \varphi_n \end{pmatrix}, \quad \varphi_{-n-1} = (-1)^n \sigma_2 \varphi_n^*, \\ \int_0^L dy \bar{\Psi} \gamma^4 i \partial_4 \Psi &= - \sum_{n=0}^{\infty} \frac{s_b \pi (2n+1)}{2L} \varphi_n^T \sigma_2 \varphi_n + \text{H.c.} \\ &(P2 - R2). \end{aligned} \quad (53)$$

If, on the other hand, we impose the periodicity condition  $P1$  then  $\Psi(y + L) = e^{i\alpha} \Psi(y)$  (corresponding to  $\cos \alpha \equiv u, \sin \alpha \equiv v$  in Table III) and we can write

$$P1: \Psi(y) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} \psi_n e^{i(2\pi n + \alpha)y/L}. \quad (54)$$

If we also impose  $R2$  then  $\psi_n$  must obey  $\psi_n = \gamma_5 \psi_n^c$  and this leads to



$$\psi_n = \begin{pmatrix} -i\sigma_2 \varphi_n^* \\ \varphi_n \end{pmatrix} \quad (P1 - R2). \quad (55)$$

In this case the bare-mass fermion term in the Lagrangian is allowed since under the orbifold twist transformation,  $\psi \rightarrow \gamma_5 \psi^c$ , the 5D fermion mass term is invariant:

$$\bar{\psi} \psi \rightarrow -\bar{\psi}^c \psi^c = \bar{\psi} \psi. \quad (56)$$

In addition, the kinetic term also generates a mass term:

$$\int_0^L dy \bar{\Psi} (i\gamma^4 \partial_4 - M) \Psi = \sum_{n=-\infty}^{\infty} \left[ 2M \varphi_n^\dagger \varphi_n - \frac{(2\pi n + \alpha)}{L} \times (\varphi_n^T \sigma_2 \varphi_n + \text{H.c.}) \right] \quad (P1 - R2). \quad (57)$$

When present, the vacuum expectation value  $\langle A_4 \rangle$  will generate an additional contribution to the mass. This important case is described in more detail in the appendix.

Finally, for the remaining  $P1 - R1$  case we find

$$\Psi(y) = s_a \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} \psi_n e^{2\pi i n y / L}; \quad \psi_{-n} = s_b \gamma_5 \psi_{n-\nu},$$

$$\int_0^L dy \bar{\Psi} \gamma^4 i \partial_4 \Psi = \sum_{n=1-\nu}^{\infty} i \frac{(2n + \nu)\pi}{L} \bar{\psi}_n \gamma_5 \psi_n \quad (P1 - R1), \quad (58)$$

where  $\nu = (1 - s_a)/2$ .

It is worth pointing out that massless fermions are present only when  $(P1 - R1)$  BC are imposed with  $s_a = +1$  or for  $(P1 - R2)$  if  $M = 0$  and  $\alpha = 0$ . Note also that the  $(P1 - R1)$  case is the only one where KK fermions are not restricted to be Majorana fermions. This is related to the fact that these BC are invariant with respect to *global*  $U(1)$  rescaling of the 5D fermion field  $\Psi(y)$ ; only for this choice fermion number remains conserved. In all cases containing  $P2$  and/or  $R2$

- (i)  $P2$ :  $\Psi(y + L) \propto \Psi^c(y)$ ,
- (ii)  $R2$ :  $\Psi(-y) \propto \Psi^c(y)$ ,

so any global  $U(1)$  symmetry is broken by the fermionic BC. Therefore the generalized BC discussed in this paper provide a natural method of constructing 4D Majorana fermions with masses of order  $1/L$ . This can be useful when building a realistic models for neutrino interactions, especially if a seesaw mechanism is also implemented.

## B. Two-Abelian fermions

The case for two-Abelian fermions can be studied along similar lines. In this case we have  $M = \text{diag}(m_1, m_2)$ ,  $T = \text{diag}(q_1, q_2)$ <sup>9</sup> and

<sup>9</sup>The  $U(1)$  gauge symmetry implies that  $[M, T] = 0$ , so therefore both  $M$  and  $T$  can be chosen diagonal.

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \quad (59)$$

We assume that masses and charges are not zero. The richest structure is allowed by the  $P1 - R2$  BC which we consider first.

### 1. $P1 - R2$ boundary conditions

This case has a special interest because it is the only one (for the two-Abelian fermion model) that allows a nonzero vacuum expectation value for  $A_4$ . The BC for the gauge fields are

$$A_N(y + L) = A_N(y), \quad A_\mu(-y) = -A_\mu(y), \quad (60)$$

$$A_4(-y) = A_4(y).$$

Concerning the fermions, the conditions  $[\mathcal{A}, \tau] = \{\mathcal{B}, \tau\} = 0$  and  $[\mathcal{A}, \mathcal{M}] = \{\mathcal{B}, \mathcal{M}\} = 0$  suggest that the cases where  $|m_1/m_2| = |q_1/q_2| = 1$  should be treated separately. This, however is not the case.

Suppose, for example, that  $m_1/m_2 = q_1/q_2 = +1$ , then the constraints on  $\mathcal{A}$  and  $\mathcal{B}$  imply  $\tilde{\Gamma} = \tilde{Y} = 0$ . In addition, the Lagrangian has a  $U(2)$  flavor symmetry that allows us to choose  $\Gamma$  diagonal and  $\tilde{Y} = \mathbb{1}$ . The boundary conditions then reduce to

$$\psi_i(y + L) = e^{i\alpha_i} \psi_i(y), \quad \psi_i(-y) = \gamma_5 \psi_i^c(y) \quad (61)$$

$$(i = 1, 2),$$

so that each flavor has an expansion of the form (54) and (55). If  $m_1/m_2 = q_1/q_2 = -1$ , then, following the discussion of Sec. II F it is convenient to introduce  $\psi_2 = (\psi_2^c)^c$  so that the new field has mass and charge  $m_2' = -m_2 = +m_1$ ,  $q_2' = -q_2 = +q_1$ ; in terms of  $\psi_1, \psi_2'$  the theory is identical to the one just considered. If the masses and charges do not satisfy  $|m_1/m_2| = |q_1/q_2| = 1$  then gauge invariance requires that the boundary conditions be again given by (61).

We conclude that with an appropriate choice of fields the two fermions decouple from each other when the boundary conditions  $(P1 - R2)$  are imposed. In this case the considerations of the previous section determine the physics of the model. In particular, for this choice of BC,  $CP$  is violated either explicitly nonzero  $\alpha_i$  or spontaneously by one-loop vacuum expectation value of  $A_4$ , see the appendix.

### 2. $P1 - R1$ boundary conditions

In this case the constraints are satisfied only when  $m_1 = m_2$  and  $q_1 = -q_2$  and provided  $\tilde{\Gamma} = \tilde{Y} = 0$ ,  $\tilde{Y} = \lambda \sigma_1$  with  $|\lambda| = 1$  and  $\Gamma = \text{diag}(e^{i\alpha}, e^{-i\alpha})$ . The freedom to re-define the global phase of the fields can then be used to set  $\lambda = 1$ , then we have

$$\psi_1(y + L) = e^{+i\alpha} \psi_1(y), \quad \psi_1(-y) = \gamma_5 \psi_2^c(y), \quad (62)$$

$$\psi_2(y + L) = e^{-i\alpha} \psi_2(y), \quad \psi_2(-y) = \gamma_5 \psi_1^c(y).$$

This can be used to eliminate  $\psi_2$ . The action then becomes twice the action for  $\psi_1$  alone, with  $\psi_1$  obeying the above periodicity condition; this case also reduces to a single-fermion model.

### 3. P2 – R1 boundary conditions

In this case the constraints are again satisfied only when  $m_1 = m_2$  and  $q_1 = -q_2$  and provided  $\tilde{\Gamma} = Y = 0$ ,  $\tilde{Y} = \lambda\sigma_1$  with  $|\lambda| = 1$  and

$$\Gamma = \begin{pmatrix} 0 & e^{i\beta} \\ e^{i\beta'} & 0 \end{pmatrix}. \quad (63)$$

The freedom to redefine the global phase of the fields can then be used to set  $\lambda = 1$ ,  $\beta' = 0$ , then we have

$$\begin{aligned} \psi_1(y+L) &= e^{+i\beta}\psi_2(y), & \psi_1(-y) &= \gamma_5\psi_2^c(y), \\ \psi_2(y+L) &= \psi_1(y), & \psi_2(-y) &= \gamma_5\psi_1^c(y). \end{aligned} \quad (64)$$

Using this to eliminate  $\psi_2$ , the action again becomes twice the action for  $\psi_1$  alone, where  $\psi_1$  obeys  $\psi_1(y) = \gamma_5\psi_1^c(-y-L)$  and  $\psi_1(y+2L) = e^{i\beta}\psi_1(y)$ . Solving these yields

$$\begin{aligned} \psi_1(y) &= \frac{1}{\sqrt{2L}} \sum e^{i\tilde{\omega}_n y} \begin{pmatrix} e^{i[\beta+(2n-1)\pi]/2} \sigma_2 \varphi_n^* \\ \varphi_n \end{pmatrix}; \\ \tilde{\omega}_n &= \frac{2\pi n + \beta}{2L}. \end{aligned} \quad (65)$$

### 4. P2 – R2 boundary conditions

These constraints require  $m_1/m_2 = -q_1/q_2 = \pm 1$ . When  $m_1 = m_2$  we again find  $\tilde{\Gamma} = Y = 0$ , and using the freedom to redefine the global phases allows us to choose  $\Gamma = e^{i\beta}\sigma_1$ ,  $\tilde{Y} = \mathbf{1}$ . The boundary conditions then become

$$\begin{aligned} \psi_1(y+L) &= e^{+i\beta}\psi_2(y), & \psi_1(-y) &= \gamma_5\psi_1^c(y), \\ \psi_2(y+L) &= e^{+i\beta}\psi_1(y), & \psi_2(-y) &= \gamma_5\psi_2^c(y). \end{aligned} \quad (66)$$

Again  $\psi_2$  can be eliminated and the action then becomes twice the action for  $\psi_1$  alone; here the constraints on  $\psi_1$  give the expansion

$$\begin{aligned} \psi_1(y) &= \frac{1}{\sqrt{2L}} \sum e^{i\tilde{\omega}_n y} \begin{pmatrix} (-1)^{n+1} i \sigma_2 \varphi_n^* \\ \varphi_n \end{pmatrix}; \\ \tilde{\omega}_n &= \frac{\pi n + \beta}{L}. \end{aligned} \quad (67)$$

When  $m_1 = -m_2$  similar arguments lead to  $\Gamma = \tilde{\Gamma} = 0$ ,  $Y = e^{i\beta}\sigma_1$ ,  $\tilde{Y} = \mathbf{1}$ , and

$$\begin{aligned} \psi_1(y) &= \frac{1}{\sqrt{2L}} \sum e^{i\tilde{\omega}_n y} \begin{pmatrix} -i \sigma_2 \varphi_n^* \\ \varphi_n \end{pmatrix}; \\ \tilde{\omega}_n &= \frac{\pi(n+1/2) + \beta}{L}. \end{aligned} \quad (68)$$

As in the previous cases we can use the BC to eliminate  $\psi_2$ ,

now in terms of a *translated*  $\psi_1$ :  $\psi_2(y) = e^{i\beta}\psi_1^c(y+L)$ . The action then reduces to that for  $\psi_1$  alone, but with the radius of the compact dimension equal to  $2L$ .

## IV. SIMPLE NON-ABELIAN CASES

### A. SU(2) models

We consider a model with SU(2) as the gauge group and where all fermions transform according to the fundamental representation. This is a pseudoreal representation generated by the Pauli matrices  $\sigma_i$ ;  $\sigma_2$  plays the role of the matrix  $S_u$  of Sec. II F.

#### 1. One doublet

When the theory contains a single SU(2) doublet,  $X, Y$ , etc. of Sec. II F are just numbers, then since the representation is pseudoreal, (34) and (35) imply  $X_i Y_i = \tilde{X}_i \tilde{Y}_i = 0$  (we drop the representation index  $u$ ), which implies that for this case either  $\Gamma$  or  $Y$  vanish (similar conclusions can be drawn for  $\tilde{\Gamma}$  and  $\tilde{Y}$ ). This leads to the possibilities listed in Table IV.

The remaining consistency condition,  $\mathcal{A}\mathcal{B} = (\mathcal{A}\mathcal{B})^\dagger$  requires  $\Gamma\tilde{\Gamma} + Y^*\tilde{Y}$  to be Hermitian and  $\Gamma^*\tilde{Y} - Y\tilde{\Gamma}$  symmetric and leads to the following constraints

$$\begin{aligned} P_{i_r} - R_{j_s}: (\tilde{U}_i^* U_i)^2 &= \begin{cases} (\tilde{\lambda}\lambda)^2 \mathbb{1}_2 & r = s, \\ -1_2 & r \neq s, \end{cases} \\ P_{1_r} - R_{2_s}: \begin{cases} (\sigma_2 \tilde{U}_2 U_1)^2 = (\lambda\tilde{\lambda})^2 & r = s, \\ \tilde{U}_2 U_1 = (\tilde{U}_2^* U_1)^T & r \neq s, \end{cases} \\ P_{2_r} - R_{1_s}: \begin{cases} (\tilde{U}_1 \sigma_2 U_2)^2 = (\lambda^* \tilde{\lambda})^2 & r = s, \\ \tilde{U}_1 U_2 = (\tilde{U}_1^* U_1)^T & r \neq s, \end{cases} \end{aligned}$$

where  $\lambda, \tilde{\lambda}$  are defined in Table V.

TABLE IV. Matrices  $\Gamma, \tilde{\Gamma}, Y, \tilde{Y}, U$  and  $\tilde{U}$  for an SU(2) model with one fermion doublet. The quantities listed satisfy  $|X_i| = |Y_j| = |\tilde{X}_k| = |\tilde{Y}_l| = 1$ , and the last column in the  $Rj$  table gives the constraints on the matrices  $\tilde{U}_i$  imposed by the consistency condition  $\mathcal{B} = \mathcal{B}^\dagger$ .

	$\Gamma$	$Y$	
$P1_a$	$X_1 U_1^\dagger$	0	
$P1_b$	0	$Y_1 U_1^T \sigma_2$	
$P2_a$	$Y_2 U_2^\dagger \sigma_2$	0	
$P2_b$	0	$X_2 U_2^T$	
	$\tilde{\Gamma}$	$\tilde{Y}$	$\tilde{U}_j$
$R1_a$	$-\tilde{X}_1 \tilde{U}_1^\dagger$	0	$\tilde{X}_1^2 \tilde{U}_1^\dagger$
$R1_b$	0	$\tilde{Y}_1 \tilde{U}_1^T \sigma_2$	$-\tilde{U}_1^\dagger$
$R2_a$	$-\tilde{Y}_2 \tilde{U}_2^\dagger \sigma_2$	0	$\tilde{Y}_2^2 \tilde{U}_2^T$
$R2_b$	0	$\tilde{X}_2 \tilde{U}_2^T$	$\tilde{U}_2^T$

TABLE V. The quantities  $\lambda, \tilde{\lambda}$  used in the definition of  $U$  and  $\tilde{U}$  for the  $SU(2)$  model with one fermion doublet.

	$P1_a$	$P1_b$	$P2_a$	$P2_b$
$\lambda$ :	$X_1$	$Y_1^*$	$Y_2$	$X_2^*$
	$R1_a$	$R1_b$	$R2_a$	$R2_b$
$\tilde{\lambda}$ :	$-\tilde{X}_1$	$\tilde{Y}_1^*$	$-\tilde{Y}_2$	$\tilde{X}_2^*$

## 2. Two $SU(2)$ doublets

We have shown in (35) that for pseudoreal representations  $\Gamma$  ( $\tilde{\Gamma}$ ) and  $Y$  ( $\tilde{Y}$ ) can be simultaneously nonzero only if at least two  $SU(2)$  pseudoreal multiplets are present; this section illustrates such a scenario. For simplicity we will restrict ourselves to the case of only two doublets.

Using then the freedom to make unitarity rotations of the doublets (which might render a nondiagonal mass matrix) it is straightforward to show that the rest of the conditions (37) have the solutions<sup>10</sup> presented in Table VI where the first matrix in the direct product acts on the flavor indices and the second on the gauge indices. We have used the fact that the general solution to  $\tilde{U}^2 = -\mathbb{1}$  is  $\tilde{U} = i\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$ , for an arbitrary (real) unit vector  $\hat{\mathbf{n}}$ ; similarly the solutions to  $\tilde{U}\tilde{U}^* = -\mathbb{1}$  are  $\tilde{U} = \pm\sigma_2$ , and, finally, the solution to  $\tilde{U}\tilde{U}^* = \mathbb{1}$  is  $\tilde{U} = \sin\tilde{\alpha} + i\cos\tilde{\alpha}\hat{\mathbf{l}} \cdot \boldsymbol{\sigma}$  with  $\tilde{\alpha}$  real and  $\hat{\mathbf{l}}$  a real unit vector perpendicular to  $\hat{\mathbf{y}}$ . We have used the freedom to make global gauge rotations to set  $\hat{\mathbf{n}} = \hat{\mathbf{z}}, \hat{\mathbf{l}} = \hat{\mathbf{x}}, \tilde{\alpha} = 0$ .

The general form of  $\mathcal{A}$  follows from (35):

$$X_i = u_i W_i, \quad Y_i = v_i W_i^* \sigma_2 \quad (70)$$

where  $W_i \in SU(2)$  and  $|u_i|^2 + |v_i|^2 = 1$ . These quantities are restricted by the conditions given in Table I, (38) and (39), Table II, but we will not study all possible cases as the results are not illuminating. The most important feature of this example is the presence of nonzero  $\Gamma$  and  $Y$  ( $\tilde{\Gamma}$  and  $\tilde{Y}$ ).

## B. $N$ $SU(3)$ triplets

In this section we consider a theory with gauge-group  $SU(3)$  containing  $N$  triplets and  $\bar{N}$  antitriplets. Using the results obtained at the end of Sec. II F we can replace all antitriplets by their charge conjugates and obtain a theory where all fermions transform as a 3 of  $SU(3)$ ; because of this we take  $\bar{N} = 0$ . In this case

$$\tau_a = \begin{pmatrix} \mathbb{1}_N \otimes \lambda_a & 0 \\ 0 & -\mathbb{1}_N \otimes \lambda_a^* \end{pmatrix}, \quad (71)$$

where  $\mathbb{1}_N$  denotes the  $N \times N$  unit matrix in flavor space and  $\{\lambda_a\}$  denote the usual Gell-Mann matrices.<sup>11</sup>

<sup>10</sup>Since there is only one representation present we drop the subscript  $u$ .

<sup>11</sup>It is worth noting that an  $SU(3)$  Hermitian matrix can be written in the form  $-(1/3)\mathbb{1}_3 + \sqrt{4/3}\hat{\ell}_a \lambda_a$  with  $\sum_a \hat{\ell}_a^2 = 1, \hat{\ell}_a = \sqrt{3}d_{abc}\hat{\ell}_b\hat{\ell}_c$  [ $d_{abc}$  denote the fully symmetric  $SU(3)$  symbols].

 TABLE VI. Matrices  $\tilde{\Gamma}, \tilde{Y}, \tilde{U}$  and the number  $\tilde{c}$  for an  $SU(2)$  model with two fermion doublets.

	$\tilde{c}$	$\tilde{\Gamma}$	$\tilde{Y}$	$\tilde{U}_1$
R1:	+1	$\cos\tilde{\theta}\mathbb{1} \otimes \mathbb{1}$	$\sin\tilde{\theta}\sigma_2 \otimes \sigma_2$	$\mathbb{1}$
	-1	$\cos\tilde{\theta}\sigma_3 \otimes \sigma_3$	$\sin\tilde{\theta}\sigma_1 \otimes \sigma_1$	$i\sigma_3$
	$\tilde{c}$	$\tilde{\Gamma}$	$\tilde{Y}$	$\tilde{U}_2$
R2:	+1	$\cos\tilde{\theta}\sigma_3 \otimes \sigma_3$	$i\sin\tilde{\theta}\sigma_1 \otimes \sigma_1$	$i\sigma_1$
	-1	$\cos\tilde{\theta}\mathbb{1} \otimes \mathbb{1}$	$\sin\tilde{\theta}\sigma_2 \otimes \sigma_2$	$-\sigma_2$

 TABLE VII. The matrices  $\Gamma, \tilde{\Gamma}, Y$  and  $\tilde{Y}$  for an  $SU(3)$  model with  $N$  triplets. The matrices  $X_i, \tilde{X}_j$  are unitary  $N \times N$  matrices restricted by the consistency conditions  $\mathcal{B} = \mathcal{B}^\dagger$  and  $\mathcal{A}\mathcal{B} = (\mathcal{A}\mathcal{B})^\dagger$  as specified in (36), Table I, (38) and Table II.

	$P1$	$P2$
$\Gamma$	$X_1 \otimes U_1^\dagger$	0
$Y$	0	$X_2 \otimes U_2^T$
	$R1$	$R2$
$\tilde{\Gamma}$	$-\tilde{X}_1 \otimes \tilde{U}_1^\dagger$	0
$\tilde{Y}$	0	$\tilde{X}_2 \otimes \tilde{U}_2^T$

If the boundary condition  $P1$  is chosen then the constraint (5) implies  $\Gamma = X_1 \otimes U_1^\dagger, Y = 0$ ; in contrast if  $P2$  is imposed then  $\Gamma = 0, Y = X_2 \otimes U_2^T$  with similar results for  $Rj$ . These results are summarized in Table VII.

## V. CONDITIONS FOR THE PRESENCE OF ZERO KK MODES

In order to extract the 4D particle content of this type of theories the standard approach is to expand the fields as Fourier series in the compact coordinate. For fermion fields the resulting Fourier modes can have 3 possible contributions to their mass: those generated by  $M$ , those generated by the  $\bar{\Psi}\partial_4\Psi$  term and, finally, those generated by  $\bar{\Psi}\langle A_4\rangle\Psi$  (whenever a nonzero vacuum expectation value is present). The scale of the last two contributions is set by  $1/L$  and is therefore relatively high. The SM light fermions are presumably much lighter than the compactification mass scale  $1/L$ , therefore in any realistic setup, the SM fermions are supposed to be zero modes, avoiding at least the large  $\bar{\Psi}\partial_4\Psi$  contribution to their mass. In considering the phenomenology of the class of 5D models discussed in this paper, it is useful to determine and discuss the general conditions that allow for the existence of such zero-modes, this is our task for this section.

Light fermions<sup>12</sup> may exist provided the boundary conditions allow zero modes and if  $\langle A_4 \rangle = 0$  [as can occur if one of the conditions (47) is not satisfied]. Specifically, we

<sup>12</sup>The terms  $\propto M$  in (1) may generate a small mass for some of the fermion zero modes.

assume that the conditions  $\chi(y) = \mathcal{A}^T \chi(y+L) = \gamma_5 \mathcal{B}^T \chi(-y)$  allow the expansion of  $\chi$  in terms of a complete set of modes,  $\chi(x, y) = \sum \chi_n(x) v_n(y)$  (examples are provided in Sec. III). Massless modes are associated with a basis function  $v_0$  that is independent of  $y$ . Writing  $\chi_0 = (\zeta^c, \zeta)^T$  and substituting into (4) and (8) gives

$$(\mathbb{1} - \mathcal{A}^*) \chi_0 = 0, \quad (\mathbb{1} - \gamma_5 \mathcal{B}^*) \chi_0 = 0. \quad (72)$$

In order to avoid having  $\chi_0 = 0$  as the only solution we must have  $\det(\mathbb{1} - \mathcal{A}^*) = \det(\mathbb{1} - \gamma_5 \mathcal{B}^*) = 0$ .

Using (3) and (9) these constraints on the light modes become

$$\begin{aligned} (\mathbb{1} - \Gamma) \zeta_L &= Y^* (\zeta_R)^c, & (\mathbb{1} + \tilde{\Gamma}) \zeta_L &= -\tilde{Y}^* (\zeta_R)^c, \\ Y \zeta_L &= (\Gamma^* - \mathbb{1}) (\zeta_R)^c, & \tilde{Y} \zeta_L &= (\tilde{\Gamma}^* - \mathbb{1}) (\zeta_R)^c. \end{aligned} \quad (73)$$

Assuming  $Y = \tilde{Y} = 0$ , the only possible solution of the above equations is  $\Gamma = \mathbb{1}$  and  $\tilde{\Gamma} = \mathbb{1}$  with  $\zeta_L = 0$  or  $\Gamma = \mathbb{1}$  and  $\tilde{\Gamma} = -\mathbb{1}$  with  $\zeta_R = 0$ . It is worth noting that this special case is the standard strategy adopted in the context of universal extra dimensions in order to construct chiral effective 4D theory.

Other solutions must be considered on a case by case basis. Note however that if  $\det \tilde{Y} \neq 0$ , then the two equations involving  $\tilde{\Gamma}$  and  $\tilde{Y}$  are equivalent: from  $\mathcal{B} = \mathcal{B}^\dagger = \mathcal{B}^{-1}$  we find  $\tilde{Y}^* \tilde{Y} = \mathbb{1} - \tilde{\Gamma}^2$  and  $\tilde{Y} \tilde{\Gamma} = \tilde{\Gamma}^* \tilde{Y}$ , so, if  $\tilde{Y}$  has an inverse, so do  $\mathbb{1} \pm \tilde{\Gamma}$ ; this also shows that  $\tilde{Y}^{*-1} (\mathbb{1} + \tilde{\Gamma}) = (\mathbb{1} - \tilde{\Gamma}^*)^{-1} \tilde{\Gamma}$  which proves the assertion. Therefore one of the constraints involving  $\tilde{\Gamma}$  and  $\tilde{Y}$  in (73) can be dropped.

From (2) and (8) one can easily find the necessary conditions which must be fulfilled for gauge-boson zero modes to exist. Denoting by  $\hat{a}, \hat{b}, \dots$  the gauge indices associated with these zero modes we find that the 4D gauge fields  $A_{\hat{a}}^\mu$  have a zero mode provided  $[\tau^{\hat{a}}, \mathcal{U}_i] = 0$  and  $[\tau^{\hat{a}}, \tilde{\mathcal{U}}_j] = 0$ . The zero mode of  $A_{\hat{a}}^4$  is present if  $[\tau^{\hat{a}}, \mathcal{U}_i] = 0$  and  $\{\tau^{\hat{a}}, \tilde{\mathcal{U}}_j\} = 0$ .

As we have already observed in Sec. III, when  $P2$  or  $R2$  boundary conditions are adopted, half of fermionic degrees of freedom is eliminated and KK modes are constrained by the Majorana condition. In particular, the fermionic zero modes may satisfy the generalized Majorana 4D condition:

$$\zeta = N C_4 (\bar{\zeta})^T, \quad (74)$$

where  $C_4$  is the 4D charge conjugation operator,<sup>13</sup> and  $N$  acts on flavor and gauge indices. In this case we can express  $\zeta$  as

$$\zeta = \begin{pmatrix} N \sigma_2 \varphi^* \\ \varphi \end{pmatrix}, \quad (75)$$

where  $\varphi$  denotes a 2-component spinor and  $\sigma_2$  acts on the

<sup>13</sup>In the Dirac representation  $C_4 = \gamma_0 \gamma_2$  while the 5D one is  $C_5 = \gamma_1 \gamma_3$ . It is useful to note that  $\gamma_5 C_5 = -i C_4$ .

Lorentz indices. Consistency of this expression requires  $NN^* = \mathbb{1}$ .

For the Majorana spinor  $\zeta$ , the conditions (72) become

$$\begin{aligned} (1 - \Gamma) \varphi + i Y^* \sigma_2 \varphi^* &= 0, & (N^* \Gamma - \Gamma^* N^*) \varphi &= 0, \\ (N^* Y^* - Y N) \varphi^* &= 0, & (N + i \tilde{Y}^*) \sigma_2 \varphi^* - \tilde{\Gamma} \varphi &= 0, \\ (N^* \tilde{\Gamma} + \tilde{\Gamma}^* N^*) \varphi &= 0, & (N^* \tilde{Y}^* + \tilde{Y} N) \varphi^* &= 0. \end{aligned} \quad (76)$$

It is useful to illustrate the above conditions by certain special cases:

- (i) If  $Y = 0$  and  $\Gamma = \mathbb{1}$  ( $\mathcal{A} = \mathbb{1}$ , so periodic fermionic fields), and  $\tilde{Y} = 0$  then it is easy to see from (76) that more than one flavor is needed to have a Majorana zero mode.
- (ii) If  $\tilde{\Gamma} = 0$ <sup>14</sup> then there is always a Majorana zero mode with  $N = -i \tilde{Y}^\dagger$ . This case is illustrated by the BC ( $P1 - R2$ ) for a single Abelian fermion, if  $u = 1, v = 0$  ( $\alpha = 0$ ) are chosen, see Table III, then  $N = -i$ . In that case the bare mass is allowed, therefore, as shown in (57), the zero KK mode is massive<sup>15</sup>.
- (iii) If  $\tilde{Y} = 0$ <sup>16</sup>,  $\Gamma^* \neq \mathbb{1}$  and  $Y$  is invertible (so charge-conjugated field appears in the periodicity BC) then again there exists a Majorana zero mode if  $N = -i Y^{-1} (\mathbb{1} - \Gamma^*) \tilde{\Gamma}^*$  and if this matrix satisfies the constraints of the last two columns in (76). For an Abelian model this again requires more than one flavor: the single-fermion case would correspond to the ( $P2 - R1$ ) BC for which, using Table III,  $\tilde{\Gamma} = s_b, Y = 1, \Gamma = \tilde{Y} = 0$ . In this case, however  $N^* \tilde{\Gamma} + \tilde{\Gamma}^* N^* = 2i$ , so that the corresponding equation in (76) implies  $\varphi = 0$ .

## A. Examples

A simple situation that allows for the presence of light modes is realized by taking  $\mathcal{A} = \mathbb{1}$  (periodic fermions), and assuming  $\det \tilde{Y} \neq 0$ , then we have

$$(\zeta_R)^c = -(\tilde{Y}^*)^{-1} (\mathbb{1} + \tilde{\Gamma}) \zeta_L, \quad (77)$$

or, equivalently,

$$\zeta = \begin{pmatrix} \tilde{\Gamma} \phi - \tilde{Y}^* i \sigma_2 \phi^* \\ \phi \end{pmatrix}, \quad (78)$$

where  $\phi$  is a two-component spinor ( $\sigma_2$  acts on Lorentz indices,  $\tilde{\Gamma}$  and  $\tilde{Y}$  on flavor indices). Using unitarity of  $\mathcal{B}$  and invariance of the mass term under the orbifold twist

<sup>14</sup>The necessary existence of  $\tilde{Y}^{-1}$  is guaranteed by the unitarity of  $\mathcal{B}$ . In this case a charge-conjugated field appears in the orbifold BC.

<sup>15</sup>For a fermion which satisfies the Majorana condition the Dirac and the Majorana mass terms are identical.

<sup>16</sup>Again the unitarity of  $\mathcal{B}$  shows that  $\tilde{\Gamma} \neq 0$ .

one can show that in this case the mass term in the Lagrangian becomes

$$\bar{\zeta} M \zeta = -2\phi^\dagger M \phi \quad (79)$$

having taken  $M$  real and diagonal. The diagonal elements of  $M$  could be chosen arbitrarily small. Note that if  $\tilde{\Gamma} = 0$  then the zero mode  $\zeta$  is a Majorana type fermion that receives its mass from the bare-mass term  $M$ .

For a specific example let us consider an  $SU(2)$  theory containing two doublets (we still assume  $\mathcal{A} = \mathbb{1}$ ). The representation is pseudoreal generated by the Pauli matrices  $\sigma_1; \sigma_2$  plays the role of the matrix  $S_u$  of Sec. II F. In this case we will write  $\zeta^T = (\psi_1, \psi_2)^T$  where  $\psi_i$  ( $i = 1, 2$ ) are doublets with the flavor index  $i$  (the gauge index is not displayed). The matrix  $\mathcal{B}$  was determined in Sec. IV A, see Table VI.

The simplest case corresponds to  $\tilde{c} = 1$  in Table VI, which we assume. This case illustrates the interesting possibility of nonzero  $\tilde{\Gamma}$  and  $\tilde{Y}$ , which can occur only if there exist at least two multiplets transforming according to the same pseudoreal representation, as was mentioned at the end of Sec. II F. We find that Table VI and (73) imply  $P_R \psi_{1,2} = \mp i \cot(\tilde{\theta}/2) \sigma_2 (P_L \psi_{2,1})^c$  (where  $\sigma_2$  acts on the gauge indices). In particular  $\psi_2$  can be expressed in terms of  $\psi_1$ :

$$\psi_2 = i \left( \frac{\cos \tilde{\theta} + \gamma_5}{\sin \tilde{\theta}} \right) \sigma_2 \psi_1^c \quad (R1, \tilde{c} = +1). \quad (80)$$

The light modes  $\zeta$  can acquire a small mass of order  $M$  provided  $\{\mathcal{B}, \mathcal{M}\} = 0$ . This can occur for  $R1$  and  $\tilde{c} = -1$  or  $R2$  and  $\tilde{c} = +1$ : in either of these cases  $M$  should satisfy  $\{\sigma_3, M\} = 0$  and  $\sigma_1 M \sigma_1 = M^*$ , so that  $M = m_1 \sigma_1 + m_2 \sigma_2, m_{1,2}$  real; the physical masses are simply  $\pm \sqrt{m_1^2 + m_2^2}$ .

Abelian examples of zero modes were briefly mentioned in Sec. III. The possibility that the gauge fields  $A^4$  acquire a vacuum expectation value contributing to the fermion mass will not be discussed in detail here.

## B. Gauge invariance

The conditions (73) need not be invariant under arbitrary  $y$ -independent gauge transformations  $\Omega, \zeta \rightarrow \Omega(x)\zeta$  [see (17)], leading to a reduction of the gauge group for the light sector. The specific constraints follow from the decomposition (30) that allows us to write  $\Omega = \text{diag}(\dots, \mathbb{1}_{d_\ell} \otimes \Omega_\ell, \dots, \mathbb{1}_{d_u} \otimes \Omega_u, \dots)$  where  $\Omega_r$  denotes a gauge transformation in the space corresponding to the irreducible representation  $r$ .

Using this we then find from (73) [or equivalently from (25) for  $y$ -independent  $\Omega$ ] that for noncomplex representations the BC are preserved by gauge transformations that obey

$$\begin{aligned} P1: [U_{1;u}, \Omega_u] &= 0, & R1: [\tilde{U}_{1;u}, \Omega_u] &= 0, \\ P2: [S_u^\dagger \cdot U_{2;u}, \Omega_u] &= 0, & R2: [S_u^\dagger \cdot \tilde{U}_{2;u}, \Omega_u] &= 0, \end{aligned} \quad (81)$$

where we use the same notation as in Sec. II F (see [12] for related arguments in the case of standard BC).

It is easy to see that the  $\Omega$  satisfying the constraints (81) form a subgroup of the original gauge group and, in general that its representation is complex. It is therefore possible to use BC to select a light sector that has both a chiral structure and a smaller gauge group. Such a breaking has future value in model building and will be investigated in a future publication.

For complex representations we find the same conditions for  $P1$  and  $R1$ , but not when  $P2$  or  $R2$  are imposed:

$$\begin{aligned} P1: [U_{1;u}, \Omega_\ell] &= 0, & R1: [\tilde{U}_{1;u}, \Omega_\ell] &= 0, \\ P2: \Omega_\ell^* &= U_{2;\ell} \Omega_\ell U_{2;\ell}^\dagger, & R2: \Omega_\ell^* &= \tilde{U}_{2;\ell} \Omega_\ell \tilde{U}_{2;\ell}^\dagger. \end{aligned} \quad (82)$$

For  $P2$  and  $R2$  these conditions cannot be satisfied by all elements of the initial gauge group (since they would then imply that the representation is noncomplex), so the gauge group of the light sector must be smaller than the initial group, and the light-sector fermions will transform according to a noncomplex representation of this subgroup.<sup>17</sup>

Let us now consider the gauge invariance of the gauge-boson light sector. As it was already mentioned earlier, the gauge fields  $A_a^\mu$  will have a zero mode provided

$$\begin{aligned} P1: +T_{\hat{a}} &= U_1 T_{\hat{a}} U_1^\dagger, & R1: +T_{\hat{a}} &= \tilde{U}_1 T_{\hat{a}} \tilde{U}_1^\dagger, \\ P2: -T_{\hat{a}}^* &= U_2 T_{\hat{a}} U_2^\dagger, & R2: -T_{\hat{a}}^* &= \tilde{U}_2 T_{\hat{a}} \tilde{U}_2^\dagger. \end{aligned} \quad (83)$$

Comparing (81) and (82) with (83), it is easy to see that both for noncomplex and for complex representations, the generators  $T_{\hat{a}}$  that correspond to zero modes generate the symmetry group of the light sector. In other words, the gauge symmetry of the zero-mode sector can be easily determined just by inspection of the massless vector bosons.

As an example let us consider here  $SU(2)$  gauge theory with a single doublet of fermions. We adopt the  $P1 - R1$  BC and choose

$$\begin{aligned} \Gamma &= \sigma_3, & Y &= 0, & U_1 &= i\sigma_3, \\ \tilde{\Gamma} &= \mathbb{1}, & \tilde{Y} &= 0, & \tilde{U}_1 &= \mathbb{1}, \end{aligned} \quad (84)$$

which is a slight modification of the example discussed at the end of Sec. II E. In that section we found that the symmetry of the light sector was completely broken due to nontrivial orbifold BC ( $\mathcal{B} \neq \mathbb{1}$ ). Here we choose  $\mathcal{B} = \mathbb{1}$  so that the  $y$ -independent gauge transformations generated by  $\sigma_3$  are allowed, as a consequence the zero mode of  $A_3^\mu$

<sup>17</sup>An example would be an  $SU(3)$  theory with fermions in the fundamental (complex) representation where the light-sector gauge group is reduced to  $SU(2)$  that has only noncomplex representations.

survives. In turn, the light fermion modes obey

$$\zeta_L = 0, \quad (\sigma_3 - \mathbb{1})(\zeta_R)^c = 0. \quad (85)$$

The light sector contains only the  $A_3^\mu$  massless gauge bosons and a right-handed, charged (and therefore massless), fermion.

## VI. SUMMARY AND CONCLUSIONS

In this paper we considered a generic gauge theory in a 5-dimensional space compactified on  $\mathbb{M}^4 \times (S_1/Z_2)$ , and studied the effects of a generalized set of boundary conditions (BC) that allow for mixing between particles and antiparticles after a translation by the size of the extra dimension or after an orbifold reflection.

We described the consequences of gauge invariance as well as the general form of the boundary conditions consistent with it. We also studied the behavior of this class of theories under 5D parity (P), charge conjugation (C) and  $CP$ . In particular we determined the conditions under  $CP$  will be violated (explicitly) by the BC as well as spontaneously, through a possible vacuum expectation value of the fifth component of the gauge fields.

We derived a simple set of conditions that determine the light-particle content of the model and the corresponding gauge subgroup, noting also the possibility that the light fermions might have chiral structure and transform under complex representations of the light-sector gauge group, even though the underlying theory is vectorlike and contains only real representations of the full gauge group. In addition we derive the conditions under which the model generates light Majorana particles.

We believe these aspects will be of relevance in constructing phenomenologically acceptable theories.

The general considerations were illustrated by many Abelian and non-Abelian examples.

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## APPENDIX: ONE ABELIAN FERMION

Here we will consider the one fermion case with (P1 – R2) BC. The fermion mass term (57), can be brought to the standard real form  $m_n^{(\text{phys})} \bar{\psi}_n \psi_n$  through the following chiral rotation<sup>18</sup>:

$$\psi_n \rightarrow \exp(i\gamma_5 \theta_n) \psi_n \quad \text{with} \quad \tan(2\theta_n) = \frac{2\pi n + \alpha}{ML}; \quad (A1)$$

$$|\theta_n| \leq \pi/4.$$

From this we find that the physical fermion masses<sup>19</sup> are

$$m_n^{(\text{phys})} = \sqrt{M^2 + \left(\frac{2\pi n + \alpha}{L}\right)^2}. \quad (A2)$$

From the orbifold conditions and from the reality of the gauge field we have the following constraints for the bosonic KK modes:

$$A_n^\mu = -A_{-n}^\mu = (A_{-n}^\mu)^*, \quad A_n^4 = +A_{-n}^4 = (A_{-n}^4)^* \quad (A3)$$

The above conditions allow us to rewrite the Lagrangian in terms of non-negative modes only. In addition one can see that  $A_{n=0}^\mu = \mathbf{Re}A_n^\mu = \mathbf{Im}A_n^4 = 0$ . Adding the gauge fixing Lagrangian,

$$\mathcal{L}_{gf} = -\frac{1}{2\xi} \left( \partial_\mu A^\mu + \xi \partial_4 A^4 \right)^2 \quad (A4)$$

the gauge-kinetic energy terms read

$$\mathcal{L}_A + \mathcal{L}_{gf} = -\frac{1}{2} \chi \square \chi + \frac{1}{2} \sum_{n=1}^{\infty} \{ B_n^\mu [(\square + \omega_n^2) g_{\mu\nu} - (1 - \xi^{-1} \partial_\mu \partial_\nu)] B_n^\nu - B_n^4 (\square + \xi \omega_n^2) B_n^4 \},$$

where  $\mathcal{L}_A = -(F_{MN})^2/4$  and where we defined the fields

$$\chi \equiv -\sqrt{L} \mathbf{Re}A_{n=0}^4, \quad B_n^\mu \equiv \sqrt{2L} \mathbf{Im}A_n^\mu, \quad (A5)$$

$$B_n^4 \equiv \sqrt{2L} \mathbf{Re}A_n^4.$$

In terms of the  $B^N$  and the rotated fermion fields defined in (A1) we obtain

$$\int_0^L dy \bar{\Psi} (i\gamma^N D_N - M) \Psi = \sum_n \bar{\psi}_n [i\not{\partial} - m_n^{(\text{phys})}] \psi_n - g\chi \sum_n \bar{\psi}_n [\sin(2\theta_n) - i\gamma_5 \cos(2\theta_n)] \psi_n - \frac{g}{\sqrt{2}} \left\{ i \sum_{k>l} \bar{\psi}_k [\cos(\theta_k - \theta_l) + i\gamma_5 \sin(\theta_k - \theta_l)] \not{B}_{k-l} \psi_l + \sum_{k>l} B_{k-l}^4 \bar{\psi}_k [\sin(\theta_k + \theta_l) - i\gamma_5 \cos(\theta_k + \theta_l)] \psi_l + \text{H.c.} \right\}, \quad (A6)$$

<sup>18</sup>The chiral rotation of the fermions induces an  $\epsilon_{\mu\nu\sigma\rho} F_{\mu\nu} F^{\sigma\rho}$  term in the Lagrangian; however, in the Abelian case considered here, this is a total derivative and therefore it can be dropped.

<sup>19</sup>In order to include contributions from nonzero vacuum expectation value of  $A_4$  one should replace  $\alpha$  by  $(\alpha - g_5 q L^{1/2} \langle A_0^4 \rangle)$ .

where  $g = g_5/\sqrt{L}$

From these expressions one can obtain the effective potential for the scalar  $\chi$ . Following [7] (including an additional factor of  $1/2$  since we are dealing with Majorana fermions) we find

$$V_{\text{eff}} = \frac{1}{4\pi^2 L^4} \text{Re}[\text{Li}_5(\zeta) + 3x\text{Li}_4(\zeta) + x^2\text{Li}_3(\zeta)], \quad (\text{A7})$$

where

$$x = ML, \quad \zeta = e^{-x+i(\alpha-gL\langle\chi\rangle)}. \quad (\text{A8})$$

The absolute minima occur at  $\alpha - gL\langle\chi\rangle = \pm\pi, \pm 3\pi, \dots$ , but this does not lead to any physical  $CP$  violation effects unless we add a second fermion with different charge and/or different  $\alpha$  (modulo  $\pi$ ), see [7].

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