

When the C in CP does not matter: Anatomy of order-4 CP eigenstates and their Yukawa interactions

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We explore the origin and Yukawa interactions of the scalars with peculiar CP properties which were recently found in a multi-Higgs model based on an order-4 CP symmetry. We relate the existence of such scalars to the enhanced freedom of defining CP , even beyond the well-known generalized CP symmetries, which arises in models with several zero-charge scalar fields. We also show that despite possessing exotic CP quantum numbers, these scalars do not have to be inert: they can have CP -conserving Yukawa interactions provided the CP acts on fermions by also mixing generations. This paper focuses on formal aspects—exposed in a pedagogical manner—and includes a brief discussion of possible phenomenological consequences.

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I. INTRODUCTION

A. Exploring exotic forms of CP violation

CP violation was extensively studied experimentally in the past half a century, yet its origin remains enigmatic [1]. CP violation may also be present in the leptonic sector, and a vigorous experimental program aims to measure it [2–6]. In the Standard Model (SM), CP violation is introduced by hand in the form of complex quark Yukawa couplings. In models with extended scalar sectors, it can arise spontaneously, as the result of the Higgs phenomenon, via CP -violating alignment of the Higgs vacuum expectation values (VEVs), and can additionally lead to CP -violating Higgs boson exchanges [7–15]. Even in the two-Higgs-doublet model (2HDM), a rather conservative extension of the minimal Higgs sector [8], the issue of CP violation has many facets [7]. New forms of CP violation were found in the past few years within 2HDM [16–20] and with more than two Higgs doublets [13,21]. Understanding how CP violation actually happens may additionally shed some light on the flavor sector hierarchy, which is often considered to be intimately intertwined with it, and on generation of the baryon asymmetry of the universe.

In short, any novel form of CP violation deserves a closer theoretical study as it may tell us something new and lead to testable predictions. The present paper is a step toward a deeper understanding of one such unusual form: spontaneous violation of the exotic CP symmetry of order-4, first proposed in [21]. This possibility requires at least three Higgs doublets and was never explored before. Since

it brings up several questions that are not easy to answer, we decided, on the way to its phenomenology, to first discuss them in a detailed and pedagogical manner.

B. Order-4 CP symmetry and its consequences

It is part of our understanding that, besides CPT symmetry, a self-consistent local quantum field theory does not uniquely define any discrete symmetry, such as C , P , and T transformations. The first general systematic study of this issue was presented long ago by Feinberg and Weinberg [22], but their analysis is restricted to the case of multiplicative phase factors. Generalization to non-Abelian discrete groups can be found in [23]. Further restrictions on phase factors involved in the discrete transformations can be found in [24,25] and in textbooks, for instance, in [1,26]. The freedom of defining the appropriate discrete transformations becomes even larger in the case of several fields with equal quantum numbers. Focusing on the CP transformation acting in the scalar sector with several fields ϕ_i , $i = 1, \dots, N$, one often considers the following generalized CP transformations (GCPs) that we denote by J_X :

$$J_X: \phi_i(\mathbf{x}, t) \xrightarrow{CP} CP\phi_i(\mathbf{x}, t)(CP)^{-1} = X_{ij}\phi_j^\dagger(-\mathbf{x}, t), \quad X_{ij} \in U(N). \quad (1)$$

From now on, we will write ϕ^* instead of ϕ^\dagger unless the scalars form a multiplet such as the electroweak doublets in multi-Higgs-doublet models. Although the details of the model building can depend on the matrix X , the common wisdom is that J_X with any unitary X can play the role of “the CP transformation” of the model. The argument is that all experimentally observable manifestations of CP

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violation can be related to CP -violating basis invariant combinations of input parameters and, being basis invariant, they do not feel the basis change induced by X [1]. The same applies to the generalized T transformations, which, in light of the CPT theorem, are also accompanied with the family-mixing matrix. If the Lagrangian and the vacuum of the theory are invariant under any generalized T symmetry, there can be no T -odd physical observable.

A nontrivial matrix X in (1) can have peculiar consequences for model building. Note that applying J_X twice leads to a pure family-space transformation,

$$\phi_i(\mathbf{x}, t) \rightarrow (CP)^2 \phi_i(\mathbf{x}, t) (CP)^{-2} = (XX^*)_{ij} \phi_j(\mathbf{x}, t). \quad (2)$$

One can bring the matrix X to a block-diagonal form [26,27], with the blocks being either 1×1 phases or 2×2 matrices of the following type:

$$\begin{pmatrix} c_\alpha & s_\alpha \\ -s_\alpha & c_\alpha \end{pmatrix} \text{ as in [27], or } \begin{pmatrix} 0 & e^{i\alpha} \\ e^{-i\alpha} & 0 \end{pmatrix} \text{ as in [26].} \quad (3)$$

This is the simplest form of X one can achieve with basis changes in the scalar space \mathbb{C}^N . If X contains at least one 2×2 block with $\alpha \neq \pi$, then $J_X^2 = XX^* \neq \mathbb{1}$, so that the CP transformation (1) is not an order-2 transformation.

Until recently, the possibility of having higher-order CP symmetry did not raise much interest. In all concrete examples considered so far, imposing such a symmetry led to models with other accidental symmetries, including CP symmetries of order 2. Thus, imposing a higher-order CP was viewed just as a compact way of defining a model [20], not as a path toward *new* models that could not be achieved through the usual “order-2 CP + family symmetry” combination. A rare exception is [28] where the higher-order CP symmetries were classified as distinct opportunities for model building.

The recent work [21], developing on an observation made in [29], gave the first concrete example of a multi-Higgs model in which the Lagrangian is symmetric only under one specific CP symmetry (1) of order-4 and its powers, without any accidental symmetry. Since this model employs three Higgs doublets, we call it CP4-3HDM and, for completeness, its scalar sector is described in Appendix A. If CP is conserved after electroweak symmetry breaking (EWSB), it leads to a remarkable consequence that the neutral physical scalars can be combined into complex fields Φ and φ that transform under CP in an unusual way,

$$\Phi(\mathbf{x}, t) \xrightarrow{CP} i\Phi(-\mathbf{x}, t), \quad \varphi(\mathbf{x}, t) \xrightarrow{CP} i\varphi(-\mathbf{x}, t). \quad (4)$$

Notice the absence of complex or Hermitian conjugation here. In other words, the fields Φ and φ are eigenstates of the CP transformation, but, unlike the CP -even and CP -odd fields one usually deals with, they are CP half-odd.

This construction brings in several questions, both fundamental and phenomenological. Does the absence of conjugation in (4) not render this transformation a form of P rather than CP transformation? Does it not lead to any internal inconsistency of the model? Can such higher-order CP symmetries be detected in the basis-invariant approach? Do these peculiar scalars lead to any phenomenological signal that cannot be compatible with any form of the “standard” CP ?

In this work, we will address some of these questions. In Sec. II a complete analysis of the scalar sector and its properties under CP is presented. The discussion starts from the standard CP transformation followed by the concept of basis dependence. Then the peculiar case of CP transformation without conjugation is explored leading ultimately to the description of the origin and properties of the CP -half-odd scalars. In Sec. III the Yukawa interaction is introduced and discussed within the context of both the standard CP symmetry and the order-4 generalized CP case. We show that by extending the idea of generalized CP symmetry to the fermion sector, it is possible to obtain models that obey the symmetry and that contain interactions between CP -half-odd scalars and fermions. The Yukawa sectors are then studied before and after electroweak symmetry breaking in Sec. IV. We summarize our findings and comment on planned work in the conclusions.

II. THE ZOO OF CP TRANSFORMATIONS IN THE SCALAR SECTOR

A. The standard CP transformation

The higher-order CP transformations have unconventional consequences, such as the CP -half-odd scalars introduced in [21]. To accompany the reader through these subtleties, we begin with a pedagogical introduction to various unusual facets of discrete transformations acting on scalar fields. Most of the material in the first half of this section is not new and can be found in textbooks such as [1] and Sec. 2 of [26]. It is presented here because it will be useful in order to clarify the origin and self-consistency of the CP -half-odd scalars, which will appear toward the end of the section. In this section, we will deal with the purely scalar sector; interaction of such scalars with fermions will be dealt with in the rest of the paper.

Let us first recap the action of the standard C and P transformations on scalars. Consider a single complex scalar field $\phi(\mathbf{x}, t)$. After quantization, it is written in terms of creation and annihilation operators that satisfy the standard commutation relations, and it reads

$$\phi(\mathbf{x}, t) = \int \tilde{d}p [a(\mathbf{p})e^{-ipx} + b^\dagger(\mathbf{p})e^{ipx}], \quad (5)$$

where $px \equiv Et - \mathbf{p}\mathbf{x}$ and $\tilde{d}p \equiv d^3p/[2E(2\pi)^3]$ [bold vectors denote three-dimensional (3D) momenta or coordinates].

The standard assignment is that the one-particle states $a^\dagger(\mathbf{p})|0\rangle$ and $b^\dagger(\mathbf{p})|0\rangle$ correspond to a particle and its antiparticle.¹ As a natural consequence of this convention, one usually postulates that the C transformation acts on operators by exchanging a and b , whereas the P transformation changes the sign of the momentum,

$$\begin{aligned} a(\mathbf{p}) &\xrightarrow{C} Ca(\mathbf{p})C^{-1} = b(\mathbf{p}), \\ b(\mathbf{p}) &\xrightarrow{C} Cb(\mathbf{p})C^{-1} = a(\mathbf{p}), \end{aligned} \quad (6)$$

$$\begin{aligned} a(\mathbf{p}) &\xrightarrow{P} Pa(\mathbf{p})P^{-1} = a(-\mathbf{p}), \\ b(\mathbf{p}) &\xrightarrow{P} Pb(\mathbf{p})P^{-1} = b(-\mathbf{p}). \end{aligned} \quad (7)$$

Clearly, both transformations, as well as their product CP , are of order 2. One then immediately sees that, in terms of the original field,

$$\phi(\mathbf{x}, t) \xrightarrow{C} \phi^*(\mathbf{x}, t), \quad \phi(\mathbf{x}, t) \xrightarrow{P} \phi(-\mathbf{x}, t). \quad (8)$$

If the Lagrangian is invariant under both transformations, they represent the symmetries of the model. Note also that if it is invariant under the global symmetry group $U(1)$ that rephases ϕ to $e^{i\alpha}\phi$ and acts trivially on other fields, then the symmetry (8) arises naturally as the nontrivial automorphism of this $U(1)$ symmetry group.

Let us now make a side remark. Although one can study how fields transform under C and P transformations separately, most phenomenologically relevant models, including the SM as well as models with extended scalar sectors beyond the SM, are chiral, and therefore, they already violate C and P separately through the gauge interactions. Discussing how scalar fields transform under these separate transformations adds little insight, but their properties under the combined transformation CP are much more relevant. CP conservation or violation does not usually follow from the gauge structure of the models, and the origin of the small CP violation observed in experiment is puzzling. So, from now on we will be studying how fields transform under the combined transformation CP , without splitting it into C and P , which is in any case not uniquely determined. Moreover, starting from the next subsection, we will suppress the arguments both of the fields and of the operators. It is always assumed that, for fields, $\mathbf{x} \rightarrow -\mathbf{x}$ and, for operators, $\mathbf{p} \rightarrow -\mathbf{p}$ under the CP transformation.

¹We stress we need to *assign* what is the antiparticle state for a given particle. In the case of a single gauge-interacting scalar field, we have no other choice but to assign $b^\dagger(\mathbf{p})|0\rangle$ as the antiparticle of $a^\dagger(\mathbf{p})|0\rangle$. If we work with two scalar fields with identical quantum numbers, the freedom to pick up the antiparticle becomes larger; see Sec. IID and the discussion after Eq. (15).

Writing $\phi(\mathbf{x}, t)$ via two real fields, $\phi = (h_1 + ih_2)/\sqrt{2}$, we see that h_1 is CP even and h_2 is CP odd. Expressing the two real fields via operators,

$$h_{1,2}(\mathbf{x}, t) = \int \tilde{d}P [a_{1,2}(\mathbf{p})e^{-iPx} + a_{1,2}^\dagger(\mathbf{p})e^{iPx}], \quad (9)$$

we identify

$$a_1 = \frac{a+b}{\sqrt{2}}, \quad a_2 = \frac{a-b}{\sqrt{2}i}, \quad (10)$$

and see that

$$a_1(\mathbf{p}) \xrightarrow{CP} a_1(-\mathbf{p}), \quad a_2(\mathbf{p}) \xrightarrow{CP} -a_2(-\mathbf{p}). \quad (11)$$

If the original Lagrangian in terms of ϕ was invariant under $U(1)$, then, in the space of h_1 and h_2 , it is invariant under $O(2) \simeq SO(2) \times \mathbb{Z}_2$, where the original $U(1)$ symmetry is mapped onto $SO(2)$, while the extra \mathbb{Z}_2 transformation is given by the sign flip of h_2 .

Certainly, if ϕ is charged under gauge interactions, so that the single-particle states $a^\dagger|0\rangle$ and $b^\dagger|0\rangle$ differ by their conserved charges, then it makes little sense to switch to the two real fields h_1 and h_2 . The conserved charge operator, together with the Hamiltonian, fixes the most convenient basis to work in. However, in the absence of any gauge interactions, working with operators a_1, a_2 or with a, b becomes just a matter of convention.

Finally, we can revert the flow of the arguments. Suppose we have a model with two real mass-degenerate fields h_1 and h_2 , one of them being CP even, and the other being CP odd. This assignment can, for example, arise as a result of rearrangement of scalar degrees of freedom after spontaneous symmetry breaking, or it can be imposed by hand on operators (11) in toy models. Then we are allowed to rewrite it in terms of a single complex field ϕ transforming under CP as $\phi(\mathbf{x}, t) \xrightarrow{CP} \phi^*(-\mathbf{x}, t)$. This remark sounds trivial, but we will see below how similar arguments lead to less familiar conclusions.

B. Basis dependence

Suppose $\phi \xrightarrow{CP} \phi^*$ as before. Let us make a basis change and define a new scalar field as $\phi' = i\phi$. Then

$$\phi' \xrightarrow{CP} i\phi^* = -(i\phi)^* = -(\phi')^*. \quad (12)$$

We stress the all-important property that CP transformation is unitary, not antiunitary, and therefore i stays intact in the first transition. The rephased complex field transforms in a different way under *the same* CP transformation. Now, writing $\phi' = (h'_1 + ih'_2)/\sqrt{2}$, we see that it is the real part, h'_1 , which is CP odd and the imaginary part, h'_2 , which is

CP even. We come to the well-known conclusion that the exact form of the CP transformation law is basis dependent.

It may happen that the model possesses *another* CP symmetry, CP' , under which ϕ transforms with an extra minus sign, while the rephased field ϕ' transforms in the standard way. Both CP and CP' can play the role of “the” CP symmetry of the model. Then, even in a fixed basis, there is no unique assignment for which the degree of freedom is CP even and which is CP odd. One must specify the particular CP transformation one wishes to test. Notice also that the product of CP and CP' , which acts by just flipping the sign $\phi \rightarrow -\phi$, is also a symmetry. This is a straightforward feature of models incorporating more than one CP symmetry. A famous example of this situation is found in the inert doublet model, a version of 2HDM with an exact \mathbb{Z}_2 symmetry that flips the sign of the second, inert, Higgs doublet [30–33]. This inert doublet gives rise to heavy neutral scalars $H \propto \text{Re}\phi_2^0$ and $A \propto \text{Im}\phi_2^0$, which are known to be of opposite CP parity but we cannot uniquely assign which is which.

In Eq. (12), we used a very specific basis change to illustrate that the standard CP transformation rule is basis dependent. A generic basis change leads to

$$\phi' \xrightarrow{CP} e^{i\alpha}(\phi')^*. \quad (13)$$

We stress once again that this is *not* a new CP transformation; it is the same transformation seen in a different basis.

C. CP transformation without conjugation

Consider now a model with two real, mass-degenerate scalars h_1 and h_2 , both of which are CP even: $h_1 \xrightarrow{CP} h_1$ and $h_2 \xrightarrow{CP} h_2$. By saying that, we assume that these scalars represent only a part of the full theory, and it is the full theory that prevents any other assignment for the CP transformation. We are then allowed to combine them into a single complex field $\phi \equiv (h_1 + ih_2)/\sqrt{2}$. By definition, it is CP even, $\phi \xrightarrow{CP} \phi$, and no conjugation is involved under the action of CP . The possibility of having CP -even complex scalar field is not new; see, for example, Eq. (23.41) in [1].

This simple math necessitates the following interpretation: the field ϕ is self-conjugate under CP and, therefore, under C , up to a possible phase factor. So is ϕ^* ; the two are not related through the CP transformation we started with. In terms of creation and annihilation operators, by using (9), we build ϕ defined as in (5) with the following operators:

$$a = \frac{a_1 + ia_2}{\sqrt{2}}, \quad b = \frac{a_1 - ia_2}{\sqrt{2}}. \quad (14)$$

Keeping in mind that these operators are mapped under CP as $a(\mathbf{p}) \xrightarrow{CP} a(-\mathbf{p})$, $b(\mathbf{p}) \xrightarrow{CP} b(-\mathbf{p})$, we see again that $a^\dagger|0\rangle$ and $b^\dagger|0\rangle$ correspond to two *different* particles, not a particle and its antiparticle, as is usually implied when writing (5). Now, since the (unbroken) gauge symmetry assigns opposite gauge charges to particles and antiparticles, we conclude that the CP -even complex scalar ϕ cannot possess any conserved nonzero gauge quantum number that would tell the particle from the antiparticle. Only when this condition is fulfilled, an ambiguity exists in defining how the charge conjugation acts in this sector.

Notice that the standard canonical quantization procedure and the computation of the Hamiltonian and momentum density in terms of operators a and b remain exactly as they are in the case of the usual complex field. This computation is based only on the algebraic manipulation of operators but does not rely on any interpretation relating the two.

D. Conjugating or not under CP is a matter of basis choice

The construction made above may seem artificial, and one may suspect that models based on respectfully looking, generalized CP transformations of the form (1) never involve such peculiarities. We will now show that they do. Just as in Sec. II B, where we showed that the presence of the minus sign in the definition of the CP transformation is a matter of basis choice, we will now show that the conjugation involved in the usual CP transformation can be “undone” in certain situations.

Consider two complex scalar fields, ϕ_1 and ϕ_2 , with definite masses transforming under CP as

$$\phi_1 \xrightarrow{CP} \phi_2^*, \quad \phi_2 \xrightarrow{CP} \phi_1^*. \quad (15)$$

If this transformation has a chance to represent a symmetry of the model, ϕ_1 and ϕ_2 must be mass degenerate and have identical gauge quantum numbers. In short, they must form a multiplet of complex scalar fields. Expressing them via operators (5) we obtain that, under the CP transformation, $a_1(\mathbf{p}) \leftrightarrow b_2(-\mathbf{p})$ and $a_2(\mathbf{p}) \leftrightarrow b_1(-\mathbf{p})$. Thus, we already encounter a situation similar to the previous subsection: the one-particle states $a_i^\dagger|0\rangle$ and $b_i^\dagger|0\rangle$, for the same i , are not particle and antiparticle of each other, despite these two operators residing inside the same field. These are, instead, two distinct particles, albeit with the same mass and opposite gauge charges.

Next, perform a $\pi/4$ rotation in the space of complex fields,

$$\begin{pmatrix} \eta \\ \xi \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad (16)$$

and observe that, upon CP , the new fields transform as $\eta \xrightarrow{CP} \eta^*$, $\xi \xrightarrow{CP} -\xi^*$, in a very conventional way. This is

also manifest at the level of creation and annihilation operators; for example, $a_1 + a_2$ residing inside the field η indeed turns into $b_1 + b_2$ upon CP transformations, just as expected for a usual complex field.

Now, among the 4 real degrees of freedom, there are two CP even, $\text{Re } \eta$ and $\text{Im } \xi$, and two CP odd, $\text{Re } \xi$ and $\text{Im } \eta$. Since they correspond to mass-degenerate fields, one can recombine fields with the same CP parity into the new complex fields $\Phi = \text{Re } \eta - i \text{Im } \xi$ and $\tilde{\Phi} = \text{Re } \xi - i \text{Im } \eta$. In this way, the new fields become, as in the previous subsection, the CP -even and CP -odd complex fields

$$\Phi \xrightarrow{CP} \Phi, \quad \tilde{\Phi} \xrightarrow{CP} -\tilde{\Phi}. \quad (17)$$

Linking η and ξ to the original complex fields, we can express the passage from ϕ_1 and ϕ_2 to Φ and $\tilde{\Phi}$ as the following transformation R :

$$R: \begin{pmatrix} \Phi \\ \tilde{\Phi} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2^* \end{pmatrix}. \quad (18)$$

This is the basis change which “undoes” the conjugation under CP .

Let us see what happens from the algebraic point of view. In Eq. (16), we pass from the (ϕ_1, ϕ_2) to the (η, ξ) description of the same space \mathbb{C}^2 in a way that preserves its complex structure (holomorphic map). This is the usual basis change belonging to $U(2)$. In Eq. (18), when passing from (ϕ_1, ϕ_2) to $(\Phi, \tilde{\Phi})$, we also map the same \mathbb{C}^2 onto itself, but via a nonholomorphic map (notice ϕ_2^* instead of ϕ_2). The transformation R cannot be represented by any $U(2)$ transformation. However, it does conserve the norm of the vector, and it belongs to the group $O(4)$ of rotations in \mathbb{R}^4 spanned by $(\text{Re}\eta, \text{Im}\eta, \text{Re}\xi, \text{Im}\xi)$ at each space-time point. Denoting the corresponding operators for the fields Φ and $\tilde{\Phi}$ as a, b and \tilde{a}, \tilde{b} , respectively, we establish the following relation:

$$\begin{pmatrix} a \\ \tilde{a} \\ b \\ \tilde{b} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \end{pmatrix}. \quad (19)$$

Promoting the basis change group from $U(2)$ to $O(4)$ is allowed only if there are no gauge quantum numbers that distinguish ϕ_i from ϕ_i^* . In this case, we are free to *define* what we call particle and antiparticle. In (15), we assumed ϕ_2 to be the fundamental field and labeled its conjugate as ϕ_2^* . But since they do not differ in their quantum numbers, we could have reversed the notation from the very start. In this case, the creation operators inside ϕ_1^* and ϕ_2^* would correspond to a particle-antiparticle pair, creation operators inside ϕ_1 and ϕ_2 —to *another* particle-antiparticle pair. The

interpretations of Eqs. (16) and (18) would also be reversed: the latter would be the normal basis change, while the former would be a nonholomorphic transformation. Let us stress once again that, when doing these manipulations, *we never redefine* the CP transformation itself. We only make the basis changes, keeping the same CP transformation all the way.²

The lesson from this discussion is the following: in the case of two complex scalar fields possessing no charges, the distinction between particles and antiparticles is blurred to such an extent that the space of fields acquires a larger intrinsic basis change freedom. All mutually orthogonal one-particle states can still be grouped into pairs of particles and antiparticles, but we have a certain freedom of defining them. As the result, the C transformation loses its importance as a transformation that maps particles to antiparticles, and in certain basis CP can look just like the P transformation. Note importantly that it is not about redefining the CP transformation; it is about the basis change freedom: *the same* CP transformation appears as the usual one in one basis and a P -resembling transformation in another.

E. Order-4 CP transformation and CP -half-odd states

The ambiguity of choosing degrees of freedom in models with two complex scalar fields not participating in gauge interactions allows one to implement even more exotic features. Consider, instead of (15), the following CP transformation:

$$J: \phi_1 \xrightarrow{CP} i\phi_2^*, \quad \phi_2 \xrightarrow{CP} -i\phi_1^*. \quad (20)$$

This transformation closely matches the CP transformation used in the CP4-3HDM; see (A3). The conjugate fields transform, naturally, as $\phi_1^* \xrightarrow{CP} -i\phi_2$, $\phi_2^* \xrightarrow{CP} i\phi_1$. The transformation defined in (20) is of order 4, as $J^2 \neq \mathbb{1}$, $J^4 = \mathbb{1}$. The CP transformation acts on the operators a_i, b_i , in the following way:

$$\begin{aligned} a_1 &\xrightarrow{CP} ib_2, & b_2 &\xrightarrow{CP} ia_1, \\ a_2 &\xrightarrow{CP} -ib_1, & b_1 &\xrightarrow{CP} -ia_2. \end{aligned} \quad (21)$$

Once again, in order for the transformation law to represent a symmetry of at least the free theory, the two fields ϕ_i and

²Let us stress that although R mixes ϕ 's and their conjugates, it is certainly *not* a Bogolyubov transformation, as it does not mix the creation and annihilation operators. The extended symmetry group allows us to mix a 's not only with other a 's but also with b 's, but never with a^\dagger or b^\dagger . The transformation R acting on a 's and b 's as in (19) is unitary, and as a result, the canonical commutation relations and the normal ordering are always preserved.

ϕ_2 must possess equal quantum numbers and be mass degenerate.

Repeating the previous analysis, we regroup the 4 real degrees of freedom in the following way:

$$\begin{pmatrix} \Phi \\ \varphi^* \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2^* \end{pmatrix}. \quad (22)$$

Notice that, in contrast to (18), we changed the definition of the second field φ . We could have done it in the previous example as well, at the expense of a slightly longer discussion. The new fields Φ and φ transform under CP in a remarkable way,

$$\Phi \xrightarrow{CP} i\Phi, \quad \varphi \xrightarrow{CP} i\varphi. \quad (23)$$

Notice again the disappearance of the conjugation. At the level of operators, one has

$$a_\Phi = \frac{a_1 + b_2}{\sqrt{2}} \xrightarrow{CP} ia_\Phi, \quad b_\Phi^\dagger = \frac{a_2^\dagger + b_1^\dagger}{\sqrt{2}} \xrightarrow{CP} ib_\Phi^\dagger, \quad (24)$$

and similarly for $a_\varphi = (a_2 - b_1)/\sqrt{2}$ and $b_\varphi^\dagger = (b_2^\dagger - a_1^\dagger)/\sqrt{2}$.

The new fields are CP eigenstates. Therefore, one can associate with them a quantum number q , which is defined modulo 4 and which generalizes the notion of CP parity. We have $q_\Phi = q_\varphi = +1$, $q_{\Phi^*} = q_{\varphi^*} = -1$. In terms of single-particle states, $b_\Phi^\dagger|0\rangle$ and $b_\varphi^\dagger|0\rangle$ have $q = +1$, while $a_\Phi^\dagger|0\rangle$ and $a_\varphi^\dagger|0\rangle$ have $q = -1$. If the model contains a CP -odd field, it must be associated with $q = 2$ (the sign is irrelevant). Although Φ and φ are eigenstates of the CP transformation, they are neither CP even nor CP odd, but rather CP half-odd. This is essentially what was found in the CP4-3HDM [21]. The origin of such states is (again) the extra freedom of basis change that one gets for two complex fields with identical masses and zero gauge couplings.

F. CP eigenstates are not compatible with conserved global charges

The constructions presented in the preceding three subsections demand the following observation.³ Consider first the situation described in Sec. II C with two mass-degenerate real fields h_1 and h_2 in the *free field limit*. The Lagrangian acquires the $O(2)$ symmetry group that via Noether's theorem leads to the conserved global charge operator

$$\begin{aligned} Q &= \int \tilde{d}p a_i^\dagger(\mathbf{p}) T_{ij} a_j(\mathbf{p}) \\ &= \int \tilde{d}p [a^\dagger(\mathbf{p})a(\mathbf{p}) - b^\dagger(\mathbf{p})b(\mathbf{p})], \end{aligned} \quad (25)$$

where $T_{ij} = i\epsilon_{ij}$ is the $SO(2)$ generator. The one-particle states $a^\dagger|0\rangle$ and $b^\dagger|0\rangle$ are eigenstates of this operator with charges ± 1 , respectively.

Had we used the usual assignment for CP , even accompanied with the phase factors, we would see $a^\dagger a \leftrightarrow b^\dagger b$ under CP , and as the result

$$(CP)Q(CP)^{-1} = -Q. \quad (26)$$

This is compatible with the notion that CP turns particles with given (global) charges into antiparticles with opposite charges. However, if we stick to the CP transformation suggested in Sec. II C, the one under which both h_1 and h_2 are even and, equivalently, $\phi \xrightarrow{CP} \phi$ without conjugation, we get $(CP)Q(CP)^{-1} = Q$. In simple words, the so-defined CP does *not* flip the sign of the global charge. One can legitimately question the validity of this definition as CP .

A similar situation takes place for two mass-degenerate complex fields ϕ_1 and ϕ_2 as described in Secs. II D and II E. Again, in the free-field limit, one has the global symmetry group $SO(4)$ of rotations among the four real degrees of freedom that leads to six charge operators Q_a , with expressions similar to the first expression in (25) but with six $SO(4)$ generators inserted. The Cartan subalgebra of $so(4)$ is two dimensional, and we need to pick up two commuting charges out of six to classify one-particle states. The exact choice of these two charge operators depends on how we combine the real degrees of freedom to build one-particle states. For example, in terms of the operators inside the complex fields, a_1 , a_2 , b_1 , b_2 , we can define two charges

$$Q_{1,2} = \int \tilde{d}p [a_1^\dagger a_1 - b_2^\dagger b_2 \pm (a_2^\dagger a_2 - b_1^\dagger b_1)]. \quad (27)$$

The physically valid definition of the CP transformation is required only to invert the signs of those charge operators that are used to classify the states. The charge operators Q_1 and Q_2 in (27) are chosen so that they indeed change signs not only under the standard CP transformation $a_i \xrightarrow{CP} b_i$ but also the GCP used in Sec. II D with $a_1 \xrightarrow{CP} b_2$ and $a_2 \xrightarrow{CP} b_1$. Thus, in the free-field theory, this definition of GCP is compatible with particles and antiparticles having opposite conserved charges.

The exotic complex fields Φ and $\tilde{\Phi}$ are also eigenstates of two commuting charge operators; they are different from those of Eq. (27) but acquire the same form if written in

³We thank the referee for raising this issue.

terms of a , b , \tilde{a} , \tilde{b} defined in Eq. (19). The problem is, however, that these charge operators *do not change signs* under the same GCP. The same conclusion holds for the order-4 GCP of Sec. II E. This is the general consequence of Φ and $\tilde{\Phi}$ being CP eigenstates: since a 's and b 's are not swapped under GCP, all combinations such as $\tilde{a}^\dagger \tilde{a}$ stay invariant.

The only way out is to demand that there be *no conserved global charge operators* whose eigenstates could be CP eigenstates. In our original model CP4 3HDM, as well as in the pedagogical examples considered above, we always require that in the full theory there be no accidental continuous symmetries and, therefore, no conserved charges. In particular, within CP4 3HDM, it is guaranteed by the self-interaction terms. In this situation, no problem raised in this subsection arises. But in the free field theory limit, when the conserved global charges appear, the nonconjugating transformation loses its status as a CP transformation. This discontinuous transition is fine, since the free theory is indeed qualitatively different from the interacting one, at least in what concerns the structure in the Hilbert space of states.

In short, a nonconjugating CP transformation is incompatible with scalars that possess conserved charges, either gauge or global. The exotic CP half-odd scalars are possible only in theories without continuous symmetries.

G. Further remarks

Before ending this section we present a few additional comments that sum up the situation for scalar fields.

First, notice that for the construction we have presented above, it is essential to have *two* complex fields: in order for the transformation (20) to work, a_i and b_i^\dagger must transform in the same way. Trying to impose a CP transformation similar to (20) for a single field, $a \xrightarrow{CP} ib$, $b \xrightarrow{CP} ia$, would lead to

$$\phi \xrightarrow{CP} \phi_{CP} = i \int \tilde{d}p [b(\mathbf{p})e^{-ipx'} - a^\dagger(\mathbf{p})e^{ipx'}], \quad (28)$$

where $x' = (t, -\mathbf{x})$. The field ϕ_{CP} cannot be written as a linear combination of ϕ and ϕ^* . As a result, the Hamiltonian density $\mathcal{H}(\phi, \phi^*)$ transforms into $\mathcal{H}(\phi_{CP}, \phi_{CP}^*) \neq \mathcal{H}(\phi, \phi^*)$. Even if one tries to construct a Hamiltonian containing both ϕ and ϕ_{CP} as in (28) as well as their conjugates, one would find that $[\phi(x), \phi_{CP}(y)]$ does not vanish at spacelike separation $(x - y)^2 < 0$. Thus, this symmetry cannot be conserved in any local causal quantum field theory.

It is nice to notice that this kind of trouble was observed by Carruthers back in 1967 [24] as an unavoidable consequence of introducing self-conjugate half-integer-isospin multiplets of boson fields. For example, for the isospin $T = 1/2$ one can define the boson field with

$T_3 = +1/2$ with operators a and b^\dagger as usual. If the conjugate state of this boson belongs to the same multiplet, with $T_3 = -1/2$, then the isospin conservation dictates that there appears an extra minus sign between the exchanged operators, just as in (28). As a result, the commutator of these two boson fields does not vanish at spacelike distances, rendering the theory nonlocal. Thus, if one has a theory with bosons sitting in an isospin doublet, then their conjugates must form another multiplet, as it happens for kaons even disregarding their charges.

Second, we stressed above that, in order for the non-holomorphic basis change to work, the scalars must have zero charges, so that neither gauge coupling nor a conserved global quantum number could distinguish a particle from an antiparticle. In the context of multi-Higgs-doublet models, and in particular the CP4-3HDM, this condition is naturally satisfied for the neutral component of the scalar fields that do not acquire the vacuum expectation values. Indeed, after EWSB, we are left with only the electromagnetic gauge group, to which the neutral Higgses do not couple. In short, there is no need to introduce CP -half-odd scalars by hand; they naturally arise in certain multidoublet models.

Third, please note that there is a certain resemblance between our treatment and the ‘‘Majorana formalism’’ developed in [34–37] for 2HDM, and to the more general approach to CP symmetries in extended scalar sectors presented in [38]. The key similarity to both works is to combine ϕ 's and ϕ^* 's into a single multiplet Φ . The effect of CP —standard or generalized—on Φ is just a transformation of Φ . This is so because Φ^* is not an independent field anymore but can be expressed as a linear map of Φ . It is this property, or to be precise, its specific realization in 2HDM, that was called in [34] the Majorana property for scalars.

Also, if one neglects the $U(1)_Y$ part of the electroweak gauge group, then the doublets ϕ_i and $\tilde{\phi}_i = i\sigma_2\phi_i^*$ transform in the same way under $SU(2)_L$ and can indeed be arbitrarily mixed [34–37] without spoiling the kinetic term and gauge interactions. This is reminiscent of our observation that when the fields ϕ possess no conserved charges, one gets an enhanced transformation freedom. The difference is that the electroweak symmetry breaking, at least in its perturbative formulation after gauge fixing, breaks the Majorana construction of [34–37], while in our case, and specifically in the CP4-3HDM, it survives and affects the CP properties of the physical neutral scalars.

Fourth, a well-known computation shows that the action of T transformation squared on any single-particle state amounts to the factor $(-1)^{2j}$, where j is its spin [26]. This leads to the famous theorem by Kramers [39] that in any system with an odd number of fermions described by a T -invariant Hamiltonian the energy eigenstates must be double degenerate. This feature is known as Kramers degeneracy. This relation, however, gets modified in the

presence of mass-degenerate multiplets [26]. When T acts on a single-particle state it can, in addition to flipping momentum and helicity, also map it to another single-particle state. The action of T^2 is then given by $(-1)^{2j} e^{2i\alpha}$, and for $\alpha = \pi/2$ it leads to a sign factor *opposite* to the standard result. This possibility requires a twofold degeneracy of mass eigenstates beyond Kramers doubling.

Fifth and final, recall that the one-particle state $b_{\Phi}^{\dagger}|0\rangle$ associated with the CP -half-odd complex field Φ is its own antiparticle, up to the extra i factor accompanying the action of CP . The one-particle state $a^{\dagger}|0\rangle$ arising from Φ^* is a *different* one-particle state and is also its own antiparticle. The presence of the extra i factor leads to the remarkable prediction that a pair of such bosons possesses the “wrong” CP parity. In their center of motion frame

$$(CP)a_{\Phi}^{\dagger}(\mathbf{p})a_{\Phi}^{\dagger}(-\mathbf{p})(CP)^{-1} = -a_{\Phi}^{\dagger}(\mathbf{p})a_{\Phi}^{\dagger}(-\mathbf{p}). \quad (29)$$

Since the operators a_{Φ} satisfy the usual commutation relations, such a pair must sit in an even partial wave state. However, its intrinsic CP parity is negative. Thus, we obtain a peculiar situation of a CP -odd pair of two identical bosons. This is something that is usually considered impossible for bosons and that was encountered so far only for Majorana fermions.

We note in passing⁴ that in a more mathematically refined formalism the quantum fields can be defined according to their transformations under pin rather than spin groups [40]. In this formalism the notions of discrete transformations must also be adjusted, and one can discuss fermion states that have “parity” $\pm i$ rather than ± 1 . It is not clear to us whether there is a deeper connection between the two phenomena.

III. COUPLING CP -HALF-ODD SCALARS TO FERMIONS

The scalar coupling with (charged) fermions is described via Yukawa interactions. In this section, we want to investigate whether this can be done for CP -half-odd scalars in the CP -conserving fashion. The textbook classification of single-fermion (pseudo)scalar bilinears being CP even and/or CP odd might lead one to suspect that it is impossible to couple them to CP -half-odd scalars and thus that such scalars must be genuinely inert. We will show, however, that this is true only if CP acts on fermions in the traditional—fermion-family-blind—way. If, instead, the CP transformation mixes fermion generations, just as it mixes scalars, then CP -conserving Yukawa interactions are allowed.

⁴We are grateful to Leonardo Pedro who brought our attention to that work.

A. Yukawa sectors with an order-2 CP symmetry

To keep the exposition pedagogical, let us start with the most general Yukawa sector with n_f fermion fields ψ_i coupled to a single neutral complex scalar field ϕ ,

$$\mathcal{L} = \bar{\psi}_i(A_{ij} + B_{ij}\gamma_5)\psi_j\phi + \bar{\psi}_i[(A^{\dagger})_{ij} - (B^{\dagger})_{ij}\gamma_5]\psi_j\phi^*, \quad (30)$$

with arbitrary complex $n_f \times n_f$ matrices A and B . We assume for the moment that the CP transformation acts on fermions in the standard way, up to an overall phase that is the same for all generations, so that bilinears get transformed as

$$\bar{\psi}_i\psi_j \xrightarrow{CP} \bar{\psi}_j\psi_i, \quad \bar{\psi}_i\gamma_5\psi_j \xrightarrow{CP} -\bar{\psi}_j\gamma_5\psi_i. \quad (31)$$

With this convention, Eq. (30) transforms into

$$\mathcal{L} = \bar{\psi}_i(A_{ij}^T - B_{ij}^T\gamma_5)\psi_j\phi_{CP} + \bar{\psi}_i[(A^*)_{ij} + (B^*)_{ij}\gamma_5]\psi_j\phi_{CP}^*. \quad (32)$$

We want this Yukawa sector to be CP conserving, which requires that we specify how the CP -transformed scalar ϕ_{CP} is related with ϕ . The conventional transformation law $\phi \xrightarrow{CP} \phi_{CP} = \phi^*$ immediately forces both matrices, A and B , to be real. Moreover, writing as usual $\phi = (h_1 + ih_2)/\sqrt{2}$ with the CP -even real field h_1 and CP -odd h_2 and decomposing Yukawa matrices into symmetric and antisymmetric parts, $A_{s,a} = (A \pm A^T)/\sqrt{2}$, $B_{s,a} = (B \pm B^T)/\sqrt{2}$, we get

$$\mathcal{L} = \bar{\psi}_i(A_s + B_a\gamma_5)_{ij}\psi_j h_1 + i\bar{\psi}_i(A_a + B_s\gamma_5)_{ij}\psi_j h_2. \quad (33)$$

In particular, for a single fermion generation, we recover the traditional expression

$$\mathcal{L} = \sqrt{2}A\bar{\psi}\psi \cdot h_1 + i\sqrt{2}B\bar{\psi}\gamma_5\psi \cdot h_2 \quad (34)$$

with real A and B .

Allowing for extra rephasing upon the CP transformation of ϕ , such as in Eq. (13), produces no effect on this construction, since it can be removed with a basis change accompanied by the overall phase change of A and B . The conclusion is that the Yukawa sector has a CP symmetry if all entries in the matrices A and B have the same phase. In particular, even in the single-generation case (34), if couplings A and B fail to satisfy $\text{Im}AB^* = 0$, then the same scalar degree of freedom will couple both to $\bar{\psi}\psi$ and to $\bar{\psi}\gamma_5\psi$. This makes the Yukawa sector CP -violating even with one fermion generation.

In Sec. IID we argued that a model with two mass-degenerate scalar fields with zero gauge quantum numbers enjoys a larger group of basis changes, which allowed us to

recast the conventional CP transformation in the form (17). Let us now see how this extended basis change affects the Yukawa sector.

We start with the general Yukawa sector as in (30) and duplicate it, with matrices A_1 and B_1 corresponding to ϕ_1 and matrices A_2 and B_2 corresponding to ϕ_2 . Assuming that the CP transformation acts on scalars as in (15), we deduce from CP conservation that $A_2^* = A_1 \equiv A$ and $B_2^* = B_1 \equiv B$. Let us focus on the part of the Lagrangian that couples scalars to $\bar{\psi}_i \psi_j$. Omitting indices, we perform the following regrouping:

$$\begin{aligned} A\phi_1 + A^*\phi_2 + \text{H.c.} &= A\phi_1 + A^*\phi_2 + A^\dagger\phi_1^* + A^T\phi_2^* \\ &= \frac{A + A^T}{\sqrt{2}} \cdot \frac{\phi_1 + \phi_2^*}{\sqrt{2}} \\ &\quad - \frac{A - A^T}{\sqrt{2}} \cdot \frac{-\phi_1 + \phi_2^*}{\sqrt{2}} + \text{H.c.} \\ &= A_s\Phi - A_a\tilde{\Phi} + \text{H.c.} \end{aligned} \quad (35)$$

Here, we used the complex scalar fields Φ and $\tilde{\Phi}$ defined in (18), whose CP parities are given in (17), and introduced symmetric and antisymmetric parts of A : $A_s = (A + A^T)/\sqrt{2}$, $A_a = (A - A^T)/\sqrt{2}$. Repeating it for matrices B , we arrive at the following Yukawa sector in terms of fields Φ and $\tilde{\Phi}$:

$$\mathcal{L} = \bar{\psi}_i [(A_s + B_a\gamma_5)_{ij}\Phi - (A_a + B_s\gamma_5)_{ij}\tilde{\Phi}] \psi_j + \text{H.c.} \quad (36)$$

The (anti)symmetric parts of coupling matrices exactly match the CP properties of Φ and $\tilde{\Phi}$. Notice also that this expression resembles (33) with the exception that the CP -even and CP -odd scalar fields are now complex and, as a consequence, we do not need to impose any phase condition on matrices A and B . Notice also that we could have constructed (36) directly from (30) just by using the known CP properties of the new scalar fields.

B. Yukawa sectors with an order-4 CP symmetry

We now turn to the order-4 CP symmetry and try to couple the CP -half-odd scalar Φ to fermions. We first assume that the CP transformation acts on fermions in the conventional way. Then, starting with (30) and using $\Phi \xrightarrow{CP} i\Phi$, we arrive at the conditions

$$iA^T = A, \quad -iB^T = B. \quad (37)$$

Applying twice, we get $A = -A$, $B = -B$, which sets both of them to zero. The only way toward a nonzero coupling of CP -half-odd scalar to fermions is to assume that the CP transformation acts nontrivially on n_f fermion generations,

$$\psi_i \xrightarrow{CP} Y_{ij}^* \cdot i\gamma^0 C \bar{\psi}_j^T, \quad Y \in U(n_f), \quad (38)$$

where, for definiteness, we selected a specific phase convention. Note that if we aim at constructing a model that preserves the so-defined CP in all sectors, we must require the fermions participating in the family mixing to be mass degenerate. With these conventions, the fermion bilinears transform as

$$\begin{aligned} \bar{\psi}_i (A_{ij} + B_{ij}\gamma_5) \psi_j &\xrightarrow{CP} \bar{\psi}_j Y_{jj}^* (A_{ij} - B_{ij}\gamma_5) Y_{ii} \psi_i \\ &= \bar{\psi}_i [Y^\dagger (A^T - B^T\gamma_5) Y]_{ij} \psi_j. \end{aligned} \quad (39)$$

Therefore, instead of (37), we arrive at the following conditions:

$$iY^\dagger A^T Y = A, \quad -iY^\dagger B^T Y = B, \quad (40)$$

and now the problem translates into finding matrices $Y \in SU(n_f)$ such that these equations have a nonzero solution.

We focus on the case of $n_f = 3$ fermion generations. First, we immediately deduce from (40) that

$$\det A = 0, \quad \text{Tr} A^k = 0, \quad k = 1, 2, 3, \quad (41)$$

and similarly for B . Next, by performing an appropriate basis change in the fermion space, we bring Y to its simplest form,

$$Y = \begin{pmatrix} e^{i\beta} & 0 & 0 \\ 0 & 0 & e^{i\alpha} \\ 0 & e^{-i\alpha} & 0 \end{pmatrix}. \quad (42)$$

In this basis, Eqs. (40) can be satisfied only with the following matrices A , B , and transformation Y :

$$\begin{aligned} \text{case 1a: } Y &= \begin{pmatrix} e^{i\beta} & 0 & 0 \\ 0 & 0 & \pm e^{-i\pi/4} \\ 0 & \pm e^{i\pi/4} & 0 \end{pmatrix}, \\ A &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & a_{23} \\ 0 & 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & b_{32} & 0 \end{pmatrix}; \end{aligned} \quad (43)$$

$$\begin{aligned} \text{case 1b: } Y &= \begin{pmatrix} e^{i\beta} & 0 & 0 \\ 0 & 0 & \pm e^{i\pi/4} \\ 0 & \pm e^{-i\pi/4} & 0 \end{pmatrix}, \\ A &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & a_{32} & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & b_{23} \\ 0 & 0 & 0 \end{pmatrix}; \end{aligned} \quad (44)$$

$$\text{case 2: } Y = \begin{pmatrix} e^{i\beta} & 0 & 0 \\ 0 & 0 & \pm i \\ 0 & \mp i & 0 \end{pmatrix},$$

$$A = \begin{pmatrix} 0 & a_{12} & a_{13} \\ \mp e^{i\beta} a_{13} & 0 & 0 \\ \pm e^{i\beta} a_{12} & 0 & 0 \end{pmatrix},$$

$$B = \begin{pmatrix} 0 & b_{12} & b_{13} \\ \pm e^{i\beta} b_{13} & 0 & 0 \\ \mp e^{i\beta} b_{12} & 0 & 0 \end{pmatrix}. \quad (45)$$

The two subcases 1a and 1b are related to each other by the permutation of the second and third fermion families. In case 2, the CP transformation is also of order-4 in the fermion space, as applying it twice gives $Y^*Y = \text{diag}(1, -1, -1)$,⁵ while in case 1 the CP transformation is, in fact, of order 8, as $Y^*Y = \text{diag}(1, -i, i)$. In both cases, the nonzero elements of the Yukawa matrices are exactly those that lead to CP -half-odd bilinear combinations. We will give explicit expressions for these bilinears in the next section.

IV. CP -HALF-ODD SCALARS COUPLED TO FERMIONS IN 3HDM

A. Yukawa sector before EWSB

In the previous section, we demonstrated that CP -half-odd scalars can in principle couple to fermions in a CP -conserving way via the usual Yukawa interactions, provided the CP acts nontrivially not only on scalars but also on fermions. Now, we want to demonstrate how this coupling arises in the CP4-3HDM, the model in which CP -half-odd scalars were first proposed [21]. Notice that in this work we do not attempt to accurately reproduce the experimentally measured values of fermion mixing and masses; we would need to break CP to achieve that. Here, we just demonstrate that there is no intrinsic inconsistency in this construction.

The Yukawa sector of the model is described as (we only show the quark sector for brevity and use the word fermion generically)

$$-\mathcal{L}_Y = \bar{Q}_{Li} \Gamma_{a,ij} d_{Rj} \phi_a + \bar{Q}_{Li} \Delta_{a,ij} u_{Rj} \tilde{\phi}_a + \phi_a^\dagger \bar{d}_{Ri} (\Gamma_{a,ij})^\dagger Q_{Lj} + \tilde{\phi}_a^\dagger \bar{u}_{Ri} (\Delta_{a,ij})^\dagger Q_{Lj}. \quad (46)$$

The fermions are chiral, and the left and right fields Q_L , d_R , and u_R can in principle transform differently under the CP transformation, with the three matrices Y_L , Y_{dR} , and Y_{uR} .

⁵Notice that this minus has nothing to do with the famous extra minus sign arising in $(CP)^{-2}\psi(x)(CP)^2 = -\psi(x)$. Here, we check how $(CP)^2$ acts on the fermion bilinears, where two such minuses cancel.

The scalar doublets transform under the CP as $\phi_a \rightarrow X_{ab}(\phi_b^\dagger)^T$. The condition that (46) is invariant under the so-constructed CP transformation is

$$Y_L^\dagger \Gamma_a^* Y_{dR} X_{ab}^* = \Gamma_b, \quad Y_L^\dagger \Delta_a^* Y_{uR} X_{ab} = \Delta_b. \quad (47)$$

We make the simplifying assumption that CP mixes the left and right fermions in the same way,

$$Y_{dR} = Y_{uR} = Y_L = Y. \quad (48)$$

This assumption is natural but not obligatory; we only want to show that even in this case one gets a consistent CP -conserving Yukawa sector.

Next, we bring the matrix X to the form (A3), and, in this basis, the conditions (47) split into

$$Y^\dagger \Gamma_1^* Y = \Gamma_1, \quad -iY^\dagger \Gamma_2^* Y = \Gamma_3, \quad iY^\dagger \Gamma_3^* Y = \Gamma_2, \\ Y^\dagger \Delta_1^* Y = \Delta_1, \quad iY^\dagger \Delta_2^* Y = \Delta_3, \quad -iY^\dagger \Delta_3^* Y = \Delta_2. \quad (49)$$

Then we make the basis change in the fermion space which brings Y to the form (42). In this basis, we again find two cases for nontrivial solutions for Γ_a and Δ_a :

(i) case 1: $\alpha = \pm\pi/4 + \pi k$,

$$\Gamma_1 = \begin{pmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & g_2^* \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & g_{23} \\ 0 & g_{32} & 0 \end{pmatrix}, \\ \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \pm g_{32}^* \\ 0 & \mp g_{23}^* & 0 \end{pmatrix}. \quad (50)$$

(ii) case 2: $\alpha = \pm\pi/2$,

$$\Gamma_1 = \begin{pmatrix} g_1 & 0 & 0 \\ 0 & g_2 & g_3 \\ 0 & -g_3^* & g_2^* \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0 & g_{12} & g_{13} \\ g_{21} & 0 & 0 \\ g_{31} & 0 & 0 \end{pmatrix}, \\ \Gamma_3 = \pm \begin{pmatrix} 0 & -e^{-i\beta} g_{13}^* & e^{-i\beta} g_{12}^* \\ e^{i\beta} g_{31}^* & 0 & 0 \\ -e^{i\beta} g_{21}^* & 0 & 0 \end{pmatrix}. \quad (51)$$

In both cases g_1 is real and all other entries are complex and independent. The expressions for Δ_a are of the same form, with parameters d_i instead of g_i and with the exchange of index $2 \leftrightarrow 3$. Thus, we have constructed the desired CP -conserving Yukawa sector based on the order-4 CP symmetry.

B. Yukawa sector after EWSB

To keep the order-4 CP symmetry after the electroweak symmetry breaking, we select the vacuum expectation value alignment $v_i = (v, 0, 0)$. This choice is symmetry protected and technically natural, and it arises in a significant part of the entire scalar potential parameter space.

For the sake of illustration, we turn to (and focus only on) charged leptons. We use the familiar notation e, μ , and τ , to label fermion generations, but we do not mean that they have the true properties of the charged leptons observed in experiment. We reiterate that in this paper we explore only the internal consistency of the construction; whether a more elaborate model with explicit or spontaneous violation of the order-4 CP can accurately describe fermion properties is left for a subsequent publication.

The charged lepton Yukawa Lagrangian is

$$-\mathcal{L}_Y = \bar{\ell}_{Li} \Gamma_{a,ij} \ell_{Rj} \phi_a + \bar{\ell}_{Ri} (\Gamma_{a,ij})^\dagger \ell_{Lj} \phi_a^*. \quad (52)$$

Here and below, ϕ_a always stands for the neutral components of the doublets: $\phi_a \equiv \phi_a^0$. Since the CP symmetry mixes the second and third generations, they must be mass degenerate. Indeed, the masses come from Γ_1 and are equal to $m_e^2 = |g_1|^2 v^2/2$ and $m_\mu^2 = m_\tau^2 = |g_2|^2 v^2/2$ (case 1) or $m_\mu^2 = m_\tau^2 = (|g_2|^2 + |g_3|^2) v^2/2$ (case 2). Notice that in case 2, when switching to the Γ_1 -diagonal basis, $\Gamma_{2,3}$ have the same form as in (51) just with redefined parameters g_{ij} .

The SM-like Higgs boson from the first doublet couples to the fermions exactly as in the SM. The neutral Higgses from the second and third doublets induce nondiagonal interactions. Let us start with case 1 given in (50) with $\alpha = -\pi/4$. Written explicitly, the Yukawa interactions with neutral scalars are

$$-\mathcal{L}_Y = \bar{\mu}_L (g_{23} \phi_2 - g_{32}^* \phi_3) \tau_R + \bar{\tau}_L (g_{32} \phi_2 + g_{23}^* \phi_3) \mu_R + \bar{\tau}_R (g_{23}^* \phi_2^* - g_{32} \phi_3^*) \mu_L + \bar{\mu}_R (g_{32}^* \phi_2^* + g_{23} \phi_3^*) \tau_L \quad (53)$$

$$= g_{23} (\bar{\mu}_L \tau_R \phi_2 + \bar{\mu}_R \tau_L \phi_3^*) + g_{32} (\bar{\tau}_L \mu_R \phi_2 - \bar{\tau}_R \mu_L \phi_3^*) + g_{23}^* (\bar{\tau}_R \mu_L \phi_2^* + \bar{\tau}_L \mu_R \phi_3) + g_{32}^* (\bar{\mu}_R \tau_L \phi_2^* - \bar{\mu}_L \tau_R \phi_3). \quad (54)$$

The last form exposes the remaining order-4 CP symmetry. For example,

$$\bar{\mu}_L \tau_R \xrightarrow{CP} -i \bar{\mu}_R \tau_L, \quad \bar{\mu}_R \tau_L \xrightarrow{CP} -i \bar{\mu}_L \tau_R, \quad (55)$$

which compensates the $\phi_2 \xrightarrow{CP} i \phi_3^*$ and $\phi_3 \xrightarrow{CP} i \phi_2$ transformation. One can further combine bilinears into CP eigenstates,

$$\begin{aligned} \bar{\mu} \tau &\xrightarrow{CP} -i \bar{\mu} \tau, & \bar{\tau} \mu &\xrightarrow{CP} i \bar{\tau} \mu, \\ \bar{\mu} \gamma_5 \tau &\xrightarrow{CP} i \bar{\mu} \gamma_5 \tau, & \bar{\tau} \gamma_5 \mu &\xrightarrow{CP} -i \bar{\tau} \gamma_5 \mu. \end{aligned} \quad (56)$$

Remarkably, the fermion bilinears shown here are CP half-odd, with quantum number $q = \pm 1$. It is also remarkable that insertion of γ_5 changes q by two units, which is the equivalent of an extra CP oddness, just as it happens in the usual case.

Finally, we switch from ϕ_2^0, ϕ_3^0 to the CP -half-odd scalars Φ, φ as shown in Appendix A. Then, the final form for the Yukawa interactions between CP -half-odd scalar and the fermions is

$$-\mathcal{L}_Y = (\bar{\mu} \tau) (g \Phi - \tilde{g} \varphi) + (\bar{\tau} \gamma_5 \mu) (\tilde{g}^* \Phi + g^* \varphi) + \text{H.c.}, \quad (57)$$

where

$$\begin{aligned} g &= \frac{c_\gamma g_{23} - s_\gamma g_{32}^*}{\sqrt{2}}, \\ \tilde{g} &= \frac{s_\gamma g_{23} + c_\gamma g_{32}^*}{\sqrt{2}}, \quad \tan 2\gamma = -\lambda_6/\lambda_5. \end{aligned} \quad (58)$$

This interaction is exactly of the type (43) for both CP -half-odd fields.

For case 2, the Yukawa interactions can be grouped as

$$-\mathcal{L}_Y = g_{12} (\bar{e}_L \mu_R \phi_2 + \bar{\tau}_R e_L \phi_3^*) + g_{13} (\bar{e}_L \tau_R \phi_2 - \bar{\mu}_R e_L \phi_3^*) + g_{21} (\bar{\mu}_L e_R \phi_2 - \bar{e}_R \tau_L \phi_3^*) + g_{31} (\bar{\tau}_L e_R \phi_2 + \bar{e}_R \mu_L \phi_3^*) + \text{H.c.} \quad (59)$$

Again, we can group bilinears into CP eigenstates, for example,

$$\begin{aligned} \bar{e} \mu + \bar{\tau} e &\xrightarrow{CP} -i (\bar{e} \mu + \bar{\tau} e), \\ \bar{e} \gamma_5 \mu + \bar{\tau} \gamma_5 e &\xrightarrow{CP} i (\bar{e} \gamma_5 \mu + \bar{\tau} \gamma_5 e). \end{aligned} \quad (60)$$

As in case 1, these bilinears are CP half-odd, and the insertion of γ_5 introduces an extra CP oddness. Finally, switching to the CP -half-odd scalars

$$-\mathcal{L}_Y = (\bar{e} \mu + \bar{\tau} e) (g_+ \Phi - \tilde{g}_+ \varphi) - (\bar{\mu} e - \bar{\tau} \tau) (\tilde{g}_-^* \Phi + g_-^* \varphi) + (\bar{e} \gamma_5 \mu - \bar{\tau} \gamma_5 e) (g_- \Phi - \tilde{g}_- \varphi) - (\bar{\mu} \gamma_5 e + \bar{e} \gamma_5 \tau) (\tilde{g}_+^* \Phi + g_+^* \varphi) + \text{H.c.}, \quad (61)$$

where we introduced the combined couplings

$$\begin{aligned}
g_+ &= \frac{(g_{12} + g_{31})c_\gamma - (g_{13}^* + g_{21}^*)s_\gamma}{2\sqrt{2}}, \\
\tilde{g}_+ &= \frac{(g_{12} + g_{31})s_\gamma + (g_{13}^* + g_{21}^*)c_\gamma}{2\sqrt{2}}, \\
g_- &= \frac{(g_{12} - g_{31})c_\gamma - (g_{13}^* - g_{21}^*)s_\gamma}{2\sqrt{2}}, \\
\tilde{g}_- &= \frac{(g_{12} - g_{31})s_\gamma + (g_{13}^* - g_{21}^*)c_\gamma}{2\sqrt{2}}, \quad (62)
\end{aligned}$$

all of them being independent. These interaction terms are exactly what is encoded in (45).

C. Discussion

The resulting Yukawa interactions (57), (61) exhibit a peculiar asymmetric pattern of couplings of the CP -half-odd scalars and their conjugates to fermion pairs. It is tempting to interpret interaction terms such as $\bar{\mu}\tau\Phi$ as a source of lepton flavor violation.

However, when reading physical processes off such interactions, one must not forget that, according to the convention adopted, the single-fermion particle and antiparticle states are linked via the conserved generalized CP transformation in the fermion space. As a result, the fermion and its antifermion creation operators belong to *different* fields, just as it was the case for scalars; see discussion after Eq. (15). Therefore, the interaction $\bar{\mu}\tau\Phi$ in case 1 describes the Φ decay to a $\mu^+\mu^-$ pair (or $\tau^+\tau^-$ transition into Φ^*), while $\bar{\tau}\mu\Phi^*$ describes the Φ^* decay to a $\tau^+\tau^-$ pair. As a result, Φ and Φ^* have different decay preferences, but since they are not antiparticles of each other, these results are hardly surprising. The situation is less trivial in case 2, where at least the lepton-flavor-violating coupling between e and μ/τ exists.

Still, one might not be fully satisfied with our convention of identifying the particle and antiparticle states for fermions. The fermions are charged and participate in the electromagnetic interactions via the standard interaction terms $\bar{\ell}_i\gamma^\mu\ell_i A_\mu$ that are diagonal in fermion flavor. Expressing them in terms of creation and annihilation operators, one sees that they correspond not only to subprocess $\mu^- \rightarrow \mu^- \gamma$ but also to $\mu^- \tau^+ \rightarrow \gamma$. One is led to the counterintuitive conclusion that despite the fact that a fermion can emit a photon without changing its flavor, it must pick up a different fermion to annihilate into a single photon.

One can revert the fermion-antifermion convention back to the usual one, in which a single fermion field contains the creation operator of a particle and the annihilation operator of its antiparticle. In this, more physically appealing case, the fermion annihilates together with its antifermion. However, in this case the Yukawa interactions (57), (61) will be manifestly CP violating, despite the fact that the CP is conserved in this model by all commonly accepted standards.

To summarize this discussion, our model reveals a surprising clash between two different conventions for particle-antiparticle assignments for charged fermions. One is “technical” and is consistent with the conserved CP symmetry, but it leads to counterintuitive transitions as $\mu^- \tau^+ \rightarrow \gamma$. The other is “physical”; it requires that at tree level particles can only annihilate with their antiparticles into a photon. But in this case one must accept that a CP -conserving model leads to manifest CP violation.

There is a third way: to simply avoid assigning who is antiparticle of whom. In this case, there is no such transformation as C parity, and the CP symmetry of order-4 the model possesses is just a peculiar symmetry linking different fields. However, it is not clear how one should phrase the physical phenomenon of CP violation and baryogenesis within this “ C -agnostic” point of view.

Yet another possibility is that it is premature to draw any phenomenological conclusion from the above observations because this model features not only a conserved CP but also the mass-degenerate μ and τ . It will be interesting to see whether in a phenomenologically relevant version of CP4-3HDM with a spontaneously broken CP any interaction of this type persists and leads to observable signals.

To this end, we note that our model bears similarity with two versions of 2HDM studied recently in [16,17], dubbed the 2HDM with “maximal CP symmetry,” and in [18]. In both cases, one imposes a higher-order GCP on the Higgs potential and then extends the symmetry to the Yukawa sector, allowing for mixing between fermion families. The first [16,17] exploits essentially the same order-4 symmetry transformation, but since it is applied to two doublets, it effectively becomes an order-2 symmetry. Indeed, applying it twice leads to the overall minus sign in the scalar sector, which can be removed by the global sign flip. The Yukawa sector turns out to be very restrictive, and upon symmetry breaking, leads to one massless fermion generation and to strong lepton flavor violation. The second work [18] asked which higher-order GCP can be imposed on 2HDM without running into immediate troubles with the quark sector. That work also confirmed that an order-4 transformation would lead to one massless fermion generation and thus was considered unphysical, but another GCP transformation with rotation angle $\alpha = \pi/3$ turned out to be compatible with the experimentally measured quark masses and mixing pattern. We notice in passing that the origin of this special value lies in one additional discrete Abelian symmetry group \mathbb{Z}_3 which exists in the 2HDM Yukawa sector. Thus, imposing GCP of order-6 is equivalent to imposing a usual CP and an order-3 family symmetry transformation.

Our CP4-3HDM differs in several important ways from those two models. First, the presence of an additional doublet renders the symmetry genuine order-4, not order-2, transformation. Second, the third doublet can acquire the VEV after EWSB making it possible to keep CP4 unbroken. It is this residual symmetry that allows us to identify

the CP -half-odd neutral scalars. Third, when CP_4 is spontaneously broken, which can easily happen in a larger part of the parameter space, the resulting fermion mass matrices do not lead to massless fermions. This is again due to the presence of a third doublet with different Yukawa matrices. Therefore, unlike 2HDM, this model may lead to a phenomenologically relevant fermion sector with interesting family-violating signatures. Moreover, these signatures do not have to be dramatic because they beat against the SM-like Yukawa structure. Building and exploring a CP_4 -3HDM with a realistic fermion sector is the next step in the exploration of this model, and we delegate this task to a future study.

Finally, we briefly comment on the possibility of CP symmetries of even higher order. First, we mention the basic group-theoretic fact that if p_1 and p_2 are two distinct primes, then $\mathbb{Z}_{p_1 p_2} \simeq \mathbb{Z}_{p_1} \times \mathbb{Z}_{p_2}$. Therefore, if, for example, the CP symmetry is of order-6, then the symmetry group can be factored into the usual CP symmetry and a family symmetry group \mathbb{Z}_3 . The only case when the CP symmetry of order p cannot be factored into a smaller-order GCP and a family symmetry is when $p = 2^k$. Thus, CP symmetries of order 8, 16, ... are in principle possible.

Explicitly constructing a model with order-8 GCP (and higher) and no other accidental symmetries is a separate task. If located purely in the scalar sector of multi-Higgs-doublet models, it must involve more than three Higgs doublets; this is because all Abelian symmetry groups of 3HDM were listed in [29] and no such example was found. One would need to repeat this procedure for 4HDM to see if there is such a model. The fact that the renormalizable potential only has quadratic and quartic terms does not contradict this possibility. Most likely, such a model will contain new complex scalars Φ_1 and Φ_3 with CP charges $q = 1$ and $q = 3$, all defined modulo 8 that would interact via quartic interactions $\Phi_1^2 \Phi_3^2$. It would be interesting to see a specific model realizing this idea.

V. CONCLUSIONS

In this paper we further explored the origin and properties of the peculiar CP -half-odd scalars recently found in the CP_4 -3HDM, a 3HDM model based on an order-4 CP symmetry [21]. The central theme is the unavoidable ambiguity—and consequently an enhanced freedom—of defining the discrete transformations C , P , and CP in models with several zero-charge fields. In this situation, the class of physically acceptable CP transformations is broader than the traditionally appreciated generalized CP . In fact, the absence of gauge charges blurs the distinction between particles and antiparticles to such an extent that the same CP transformation can resemble a P transformation through a mere basis change. Although some previous publications hinted at this formal possibility, no specific example of such a construction was known. We found and explored such examples.

To accompany the reader through the meander of subtleties, we gave in this paper a pedagogical presentation, through examples, of the salient features for C , P , and CP symmetries acting on scalars. We also linked some of our material to results obtained by others in different approaches to CP symmetries.

In the second part of the paper, we showed that CP -half-odd scalars can be coupled to fermions via the usual Yukawa interactions in the CP -conserving way, provided the CP acts on fermions as a family-mixing generalized CP transformation. We found two classes of Yukawa matrices for the case of three fermion generations. Phenomenologically, it implies that the CP -half-odd scalars introduced in CP_4 -3HDM do not have to be inert after all.

The purpose of this work was to show the internal consistency of CP -half-odd scalars and of their Yukawa interactions. To this end, when analyzing CP_4 -3HDM, we deliberately selected the vacuum alignment that conserves the order-4 CP symmetry. Certainly, the model with the exact CP symmetry cannot reproduce the experimentally observed fermion masses and mixing. Given the results obtained in this work, one is now led to ask whether a similar model, based on the spontaneous or explicit breaking of the order-4 CP symmetry, can accurately reproduce the flavor sector and whether it will be more economical than other model-building attempts. This investigation is delegated to a future publication.

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APPENDIX: SCALAR SECTOR OF THE CP_4 -3HDM

The Higgs potential in the CP_4 -3HDM considered in [21] is $V = V_0 + V_1$, where

$$\begin{aligned}
 V_0 = & -m_{11}^2(\phi_1^\dagger\phi_1) - m_{22}^2(\phi_2^\dagger\phi_2 + \phi_3^\dagger\phi_3) + \lambda_1(\phi_1^\dagger\phi_1)^2 \\
 & + \lambda_2[(\phi_2^\dagger\phi_2)^2 + (\phi_3^\dagger\phi_3)^2] + \lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2 + \phi_3^\dagger\phi_3) \\
 & + \lambda'_3(\phi_2^\dagger\phi_2)(\phi_3^\dagger\phi_3) \\
 & + \lambda_4[(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) + (\phi_1^\dagger\phi_3)(\phi_3^\dagger\phi_1)] \\
 & + \lambda'_4(\phi_2^\dagger\phi_3)(\phi_3^\dagger\phi_2), \tag{A1}
 \end{aligned}$$

with all parameters being real, and

$$V_1 = \lambda_5(\phi_3^\dagger\phi_1)(\phi_2^\dagger\phi_1) + \frac{\lambda_6}{2}[(\phi_2^\dagger\phi_1)^2 - (\phi_1^\dagger\phi_3)^2] \\ + \lambda_8(\phi_2^\dagger\phi_3)^2 + \lambda_9(\phi_2^\dagger\phi_3)(\phi_2^\dagger\phi_2 - \phi_3^\dagger\phi_3) \\ + \text{H.c.}, \quad (\text{A2})$$

with real λ_5 , λ_6 and complex λ_8 , λ_9 . This potential is invariant under the generalized CP transformation J_X defined in (1), with

$$X = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{pmatrix}. \quad (\text{A3})$$

A key observation is that J_X is an order-4 transformation,

$$J_X^2 = XX^* = \text{diag}(1, -1, -1) \neq \mathbb{1}, \\ J_X^4 = \mathbb{1} \equiv \text{diag}(1, 1, 1). \quad (\text{A4})$$

For generic values of the coefficients, this potential has no other Higgs family or CP symmetries apart from powers of J_X [29]. Equations (A1) and (A2) define the most general renormalizable potential to which one arrives starting from any 3HDM invariant under an order-4 CP and applying basis change transformations to reduce the number of complex coefficients.

Next, we select the CP -conserving vacuum alignment: $\langle\phi_1^0\rangle = v/\sqrt{2}$, $\langle\phi_2\rangle = \langle\phi_3\rangle = 0$. For physical scalars, we get the SM-like Higgs with mass $m_{h_{\text{SM}}}^2 = 2\lambda_1 v^2 = 2m_{11}^2$ and a pair of degenerate charged Higgses with $m_{H^\pm}^2 = \lambda_3 v^2/2 - m_{22}^2$. In the neutral scalar sector, the mass matrices for real $h_{2,3}$ and imaginary $a_{2,3}$ components of $\phi_{2,3}^0$ split,

$$M_{h_2, h_3} = \begin{pmatrix} a+b & c \\ c & a-b \end{pmatrix}, \quad M_{a_2, a_3} = \begin{pmatrix} a-b & -c \\ -c & a+b \end{pmatrix}, \\ a = \frac{1}{2}v^2(\lambda_3 + \lambda_4) - m_{22}^2 = m_{H^\pm}^2 + \frac{1}{2}v^2\lambda_4, \\ b = \frac{1}{2}v^2\lambda_6, \quad c = \frac{1}{2}v^2\lambda_5, \quad (\text{A5})$$

and lead to the same physical scalar spectrum in both spaces,

$$M^2 = a + \sqrt{b^2 + c^2}, \quad m^2 = a - \sqrt{b^2 + c^2}. \quad (\text{A6})$$

The diagonalization of both mass matrices is performed by a rotation with the angle α defined as $\tan 2\alpha = \lambda_5/\lambda_6$, but it proceeds in the opposite directions for h 's and a 's. The two heavier scalars H and A and the two lighter scalars h and a are related to initial fields as

$$\begin{pmatrix} H \\ h \end{pmatrix} = \begin{pmatrix} c_\alpha & s_\alpha \\ -s_\alpha & c_\alpha \end{pmatrix} \begin{pmatrix} h_2 \\ h_3 \end{pmatrix}, \\ \begin{pmatrix} a \\ A \end{pmatrix} = \begin{pmatrix} c_\alpha & s_\alpha \\ -s_\alpha & c_\alpha \end{pmatrix} \begin{pmatrix} a_2 \\ a_3 \end{pmatrix}. \quad (\text{A7})$$

Note that upon (A7), ϕ_2^0 and ϕ_3^0 transform to

$$c_\alpha\phi_2^0 + s_\alpha\phi_3^0 = \frac{1}{\sqrt{2}}(H + ia), \\ -s_\alpha\phi_2^0 + c_\alpha\phi_3^0 = \frac{1}{\sqrt{2}}(h + iA). \quad (\text{A8})$$

The real neutral fields H , A , h , a are not CP eigenstates,

$$H \xrightarrow{CP} A, \quad A \xrightarrow{CP} -H, \quad h \xrightarrow{CP} -a, \quad a \xrightarrow{CP} h. \quad (\text{A9})$$

One can combine them into neutral fields, $\Phi = (H - iA)/\sqrt{2}$, $\varphi = (h + ia)/\sqrt{2}$, which are CP and mass eigenstates,

$$\Phi \xrightarrow{CP} i\Phi, \quad \varphi \xrightarrow{CP} i\varphi. \quad (\text{A10})$$

One can then quantify the CP properties with the global quantum number q defined modulo 4 and assign $q = +1$ to Φ , φ , and $q = -1$ to their conjugate fields. All other neutral fields are either CP odd, $q = +2$, or CP even, $q = 0$. This quantum number can also be associated with single-particle states as defined in Sec. II E. Since CP is a good symmetry of the Lagrangian and of the vacuum, it commutes with the Hamiltonian. Therefore, in any transition between initial and final states with definite q , this quantum number is conserved.

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