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Conditions for *CP* violation in the general two-Higgs-doublet model

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The most general Higgs potential of the two-Higgs-doublet model (2HDM) contains three squared-mass parameters and seven quartic self-coupling parameters. Among these, one squared-mass parameter and three quartic coupling parameters are potentially complex. The Higgs potential explicitly violates *CP* symmetry if and only if no choice of basis exists in the two-dimensional Higgs flavor space in which all the Higgs potential parameters are real. We exhibit four independent potentially complex invariant (basis-independent) combinations of mass and coupling parameters and show that the reality of all four invariants provides the necessary and sufficient conditions for an explicitly *CP*-conserving 2HDM scalar potential. Additional potentially complex invariants can be constructed that depend on the Higgs field vacuum expectation values (vevs). We demonstrate how these can be used together with the vev-independent invariants to distinguish between explicit and spontaneous *CP* violation in the Higgs sector.

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I. INTRODUCTION

The standard model (SM) posits the existence of a single complex hypercharge-one Higgs doublet [1]. Because of the form of the Higgs potential, one component of this Higgs scalar acquires a vacuum expectation value (vev) and the $SU(2) \times U(1)$ electroweak symmetry is spontaneously broken to $U(1)_{EM}$. Hermiticity requires that the parameters of the SM Higgs potential are real. Consequently, the resulting bosonic sector of the electroweak theory is *CP* conserving. *CP* violation enters through the Yukawa couplings of the Higgs field to fermions. Although there are many potentially complex parameters in the Higgs couplings to three generations of quarks and leptons, one can redefine the fermion fields (to absorb unphysical phases). The end result is one *CP*-violating parameter—the Cabibbo-Kobayashi-Maskawa angle [2].

There are a number of motivations for considering extended Higgs sectors. For example, the minimal supersymmetric extension of the standard model (MSSM) requires two complex Higgs doublets [3]. In this paper, we consider the most general two-Higgs-doublet extension of the standard model. This model possesses two identical complex, hypercharge-one Higgs doublets. In contrast to the standard model, the scalar Higgs potential of the two-Higgs-doublet model (2HDM) contains potentially complex parameters [4]. Consequently, the purely bosonic sector can exhibit explicit *CP* violation (prior to the introduction of the fermions and the attendant complex Higgs-fermion Yukawa couplings). However as above, not all complex phases are physical. In this paper, we exhibit the necessary and sufficient conditions for an explicitly *CP*-conserving 2HDM scalar potential.

The procedure for determining whether the Higgs potential explicitly violates *CP* is in principle straightforward. The Higgs potential parameters are initially defined with respect to two identical Higgs fields Φ_1 and Φ_2. However, one can always choose to change the basis (in the two-dimensional Higgs "flavor" space) by defining two new (orthonormal) linear combinations of Φ_1 and Φ_2. In this new basis, all the Higgs potential parameters are modified. The Higgs potential is explicitly *CP* violating if and only if no choice of basis exists in which all the Higgs potential parameters are simultaneously real.[1] If (at least) one basis choice exists in which all Higgs potential parameters are real, then the Higgs potential is *explicitly CP* conserving. Henceforth, we designate any such basis as a *real basis*. *CP* violation in the scalar sector might still arise if the scalar field vacuum is not time-reversal invariant. In this case, *CP* is spontaneously broken [5].

Given an arbitrary Higgs potential, it may not be possible to determine by inspection whether a real basis exists. Since there exist four potentially complex parameters in the Higgs potential, one must in general solve a set of four nonlinear equations (requiring that these four parameters are real in some specific basis to be determined). Thus, we propose another technique for answering the question of whether a special basis exists in which all Higgs potential parameters are real. Our procedure makes use of the technology introduced in Ref. [6] based on invariant combinations of Higgs potential parameters. By definition, these invariants are basis-independent quantities; i.e., they do not depend on the initial basis choice for Φ_1 and Φ_2. We then search for potentially complex invariants.

Four potentially complex (basis-independent) invariants govern the *CP* property of the 2HDM scalar potential. If any one of these four invariants possesses a nonzero imaginary part, then the 2HDM scalar potential is explicitly *CP* violating. *CP* is explicitly conserved if and only if all four invariants are real. In the latter case, a real basis must exist (even though an explicit form for the transformation that produces such a basis is not determined). Two of the

[1]We find it convenient and illuminating to give an explicit proof of this oft-stated result in Appendix A.

invariants were found by diagrammatic techniques in Ref. [6]. Recently, three of the four invariants were also employed in [7]. Other earlier simple (basis-dependent) conditions proposed for the existence of explicit *CP* violation in the Higgs potential [8,9] turn out to be sufficient but *not* necessary for an explicitly *CP*-conserving Higgs potential.

Finally, we note that in the discussion above, we have not addressed the question of the minimization of the Higgs potential. This determines the vevs of the two Higgs fields,[2] which are basis-dependent quantities. The two vevs can in general be complex, although one can absorb these complex phases by phase redefinitions of the individual scalar fields [10]. As shown in Appendix F, the Higgs sector is fully *CP* conserving if and only if there exists a real basis in which the Higgs vacuum expectation values are simultaneously real. The latter can be established by examining three additional invariants (initially introduced in Ref. [11]) that depend explicitly on the vevs.

In Sec. II, the basis-independent formalism for the 2HDM developed in Ref. [6] is reviewed. In Sec. III, we exhibit a set of four independent potentially complex invariants constructed from the Higgs sector parameters. We then prove that the imaginary parts of these four invariants vanish if and only if the 2HDM scalar potential explicitly conserves the *CP* symmetry. The proof of this theorem relies on a number of important lemmas that are proved in Appendixes C and D. The power of this theorem is demonstrated by exhibiting three simple 2HDM models with complex parameters that are *CP* conserving. In Sec. IV we provide some insight into how the set of four complex invariants was discovered by surveying all potentially complex nth-order invariants for $n \leq 6$. The manifest reality of all invariants of order three or less is demonstrated explicitly in Appendix E. Thus, one must search for invariants of order $n \geq 4$ to find candidates that are potentially complex. From the results of our survey, we deduce a number of general features of the potentially complex invariants of arbitrary order. The question of spontaneous *CP* violation in the 2HDM is treated in Sec. V. To determine whether an explicitly *CP*-conserving Higgs potential exhibits spontaneous *CP* violation, one must additionally consider basis-independent quantities, initially introduced in Ref. [11], that depend on the Higgs vevs. Finally, a brief discussion of future directions and concluding remarks are given in Sec. VI.

II. THE HIGGS POTENTIAL OF THE TWO-HIGGS-DOUBLET MODEL

Consider the most general two-Higgs-doublet extension of the standard model [1,12]. Let Φ_1 and Φ_2 denote two complex $Y = 1$, $\mathrm{SU}(2)_L$ doublet scalar fields. The most general $\mathrm{SU}(2)_L \times \mathrm{U}(1)_Y$ invariant scalar potential is given by (see, e.g., Ref. [13])

$$\begin{aligned}\mathcal{V} = {}& m_{11}^2 \Phi_1^\dagger \Phi_1 + m_{22}^2 \Phi_2^\dagger \Phi_2 - [m_{12}^2 \Phi_1^\dagger \Phi_2 + \mathrm{H.c.}] \\ & + \frac{1}{2}\lambda_1 (\Phi_1^\dagger \Phi_1)^2 + \frac{1}{2}\lambda_2 (\Phi_2^\dagger \Phi_2)^2 + \lambda_3 (\Phi_1^\dagger \Phi_1) \\ & \times (\Phi_2^\dagger \Phi_2) + \lambda_4 (\Phi_1^\dagger \Phi_2)(\Phi_2^\dagger \Phi_1) + \bigg\{\frac{1}{2}\lambda_5 (\Phi_1^\dagger \Phi_2)^2 \\ & + [\lambda_6 (\Phi_1^\dagger \Phi_1) + \lambda_7 (\Phi_2^\dagger \Phi_2)]\Phi_1^\dagger \Phi_2 + \mathrm{H.c.}\bigg\}, \end{aligned} \tag{1}$$

where m_{11}^2, m_{22}^2, and $\lambda_1, \ldots, \lambda_4$ are real parameters and m_{12}^2, λ_5, λ_6 and λ_7 are potentially complex parameters. We assume that the parameters of the scalar potential are chosen such that the minimum of the scalar potential respects the $\mathrm{U}(1)_{\mathrm{EM}}$ gauge symmetry. Then, the scalar field vacuum expectation values are of the form

$$\langle \Phi_1 \rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \qquad \langle \Phi_2 \rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_2 e^{i\xi} \end{pmatrix}, \tag{2}$$

where v_1 and v_2 are real and non-negative, $0 \leq |\xi| \leq \pi$, and

$$v^2 \equiv v_1^2 + v_2^2 = \frac{4m_W^2}{g^2} = (246\ \mathrm{GeV})^2. \tag{3}$$

In writing Eq. (2), we have used a global $\mathrm{U}(1)_Y$ hypercharge rotation to eliminate the phase of v_1.

Since the scalar doublets Φ_1 and Φ_2 have identical $\mathrm{SU}(2) \times \mathrm{U}(1)$ quantum numbers, one is free to define two orthonormal linear combinations of the original scalar fields. The parameters appearing in Eq. (1) depend on a particular *basis choice* of the two scalar fields. Relative to an initial (generic) basis choice, the scalar fields in the new basis are given by $\Phi' = U\Phi$ [6], where U is a U(2) matrix[3]:

$$U = e^{i\psi}\begin{pmatrix} \cos\theta & e^{-i\xi}\sin\theta \\ -e^{i\chi}\sin\theta & e^{i(\chi-\xi)}\cos\theta \end{pmatrix}. \tag{4}$$

Note that the phase ψ has no effect on the scalar potential parameters, since this corresponds to a global hypercharge rotation.

With respect to the new Φ'-basis, the scalar potential takes on the same form given in Eq. (1) but with new coefficients $m_{ij}'^2$ and λ_j'. For the general U(2) transformation of Eq. (4) with $\Phi' = U\Phi$, the scalar potential parameters ($m_{ij}'^2$, λ_i') are related to the original parameters (m_{ij}^2, λ_i) by

$$m_{11}'^2 = m_{11}^2 c_\theta^2 + m_{22}^2 s_\theta^2 - \mathrm{Re}(m_{12}^2 e^{i\xi}) s_{2\theta}, \tag{5}$$

[2]We shall always assume that the Higgs potential parameters are chosen such that the scalar minimum of interest preserves $\mathrm{U}(1)_{\mathrm{EM}}$.

[3]This U(2) transformation has also been recently exploited in Ref. [10].

$$m'^2_{22} = m^2_{11}s^2_\theta + m^2_{22}c^2_\theta + \mathrm{Re}(m^2_{12}e^{i\xi})s_{2\theta}, \tag{6}$$

$$m'^2_{12}e^{i\chi} = \frac{1}{2}(m^2_{11} - m^2_{22})s_{2\theta} + \mathrm{Re}(m^2_{12}e^{i\xi})c_{2\theta} + i\,\mathrm{Im}(m^2_{12}e^{i\xi}), \tag{7}$$

and

$$\lambda'_1 = \lambda_1 c^4_\theta + \lambda_2 s^4_\theta + \frac{1}{2}\lambda_{345}s^2_{2\theta} + 2s_{2\theta}[c^2_\theta\,\mathrm{Re}(\lambda_6 e^{i\xi}) + s^2_\theta\,\mathrm{Re}(\lambda_7 e^{i\xi})], \tag{8}$$

$$\lambda'_2 = \lambda_1 s^4_\theta + \lambda_2 c^4_\theta + \frac{1}{2}\lambda_{345}s^2_{2\theta} - 2s_{2\theta}[s^2_\theta\,\mathrm{Re}(\lambda_6 e^{i\xi}) + c^2_\theta\,\mathrm{Re}(\lambda_7 e^{i\xi})], \tag{9}$$

$$\lambda'_3 = \frac{1}{4}s^2_{2\theta}[\lambda_1 + \lambda_2 - 2\lambda_{345}] + \lambda_3 - s_{2\theta}c_{2\theta}\,\mathrm{Re}[(\lambda_6 - \lambda_7)e^{i\xi}], \tag{10}$$

$$\lambda'_4 = \frac{1}{4}s^2_{2\theta}[\lambda_1 + \lambda_2 - 2\lambda_{345}] + \lambda_4 - s_{2\theta}c_{2\theta}\,\mathrm{Re}[(\lambda_6 - \lambda_7)e^{i\xi}], \tag{11}$$

$$\lambda'_5 e^{2i\chi} = \frac{1}{4}s^2_{2\theta}[\lambda_1 + \lambda_2 - 2\lambda_{345}] + \mathrm{Re}(\lambda_5 e^{2i\xi}) + ic_{2\theta}\,\mathrm{Im}(\lambda_5 e^{2i\xi}) - s_{2\theta}c_{2\theta}\,\mathrm{Re}[(\lambda_6 - \lambda_7)e^{i\xi}] - is_{2\theta}\,\mathrm{Im}[(\lambda_6 - \lambda_7)e^{i\xi})], \tag{12}$$

$$\lambda'_6 e^{i\chi} = -\frac{1}{2}s_{2\theta}[\lambda_1 c^2_\theta - \lambda_2 s^2_\theta - \lambda_{345}c_{2\theta} - i\,\mathrm{Im}(\lambda_5 e^{2i\xi})] + c_\theta c_{3\theta}\,\mathrm{Re}(\lambda_6 e^{i\xi}) + s_\theta s_{3\theta}\,\mathrm{Re}(\lambda_7 e^{i\xi}) + ic^2_\theta\,\mathrm{Im}(\lambda_6 e^{i\xi}) + is^2_\theta\,\mathrm{Im}(\lambda_7 e^{i\xi}), \tag{13}$$

$$\lambda'_7 e^{i\chi} = -\frac{1}{2}s_{2\theta}[\lambda_1 s^2_\theta - \lambda_2 c^2_\theta + \lambda_{345}c_{2\theta} + i\,\mathrm{Im}(\lambda_5 e^{2i\xi})] + s_\theta s_{3\theta}\,\mathrm{Re}(\lambda_6 e^{i\xi}) + c_\theta c_{3\theta}\,\mathrm{Re}(\lambda_7 e^{i\xi}) + is^2_\theta\,\mathrm{Im}(\lambda_6 e^{i\xi}) + ic^2_\theta\,\mathrm{Im}(\lambda_7 e^{i\xi}), \tag{14}$$

where

$$\lambda_{345} \equiv \lambda_3 + \lambda_4 + \mathrm{Re}(\lambda_5 e^{2i\xi}). \tag{15}$$

These equations exhibit the following features. If $m^2_{11} = m^2_{22}$ and $m^2_{12} = 0$ in some basis then these two conditions are true in all bases. Likewise, if $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ in some basis then these latter two conditions are true in all bases.

We noted previously that the parameters m^2_{12}, λ_5, λ_6 and λ_7 are potentially complex. We now pose the following question: does there exist a so-called real basis in which all the scalar potential parameters are real? In general, the existence of a real basis cannot be ascertained by inspection. In particular, starting from an arbitrary basis, it may be quite difficult to determine whether or not there is a choice of θ, χ, ξ above such that all the primed parameters are real. However, in this paper we will show, using the basis-independent techniques described in Ref. [6], that there is a straightforward procedure for determining whether a real basis exists. To accomplish this goal, we write the scalar Higgs potential of the 2HDM following Refs. [4,6]:

$$\mathcal{V} = Y_{a\bar{b}}\Phi^\dagger_{\bar{a}}\Phi_b + \frac{1}{2}Z_{a\bar{b}c\bar{d}}(\Phi^\dagger_{\bar{a}}\Phi_b)(\Phi^\dagger_{\bar{c}}\Phi_d), \tag{16}$$

where the indices a, $\bar{b}$, c and $\bar{d}$ run over the two-dimensional Higgs flavor space and

$$Z_{a\bar{b}c\bar{d}} = Z_{c\bar{d}a\bar{b}}. \tag{17}$$

Hermiticity of $\mathcal{V}$ implies that

$$Y_{a\bar{b}} = (Y_{b\bar{a}})^*, \qquad Z_{a\bar{b}c\bar{d}} = (Z_{b\bar{a}d\bar{c}})^*. \tag{18}$$

Under a global U(2) transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$ (and $\Phi^\dagger_{\bar{a}} \to \Phi^\dagger_{\bar{b}}U^\dagger_{b\bar{a}}$), where $U^\dagger_{b\bar{a}}U_{a\bar{c}} = \delta_{b\bar{c}}$, and the tensors Y and Z transform covariantly: $Y_{a\bar{b}} \to U_{a\bar{c}}Y_{c\bar{d}}U^\dagger_{d\bar{b}}$ and $Z_{a\bar{b}c\bar{d}} \to U_{a\bar{e}}U^\dagger_{f\bar{b}}U_{c\bar{g}}U^\dagger_{h\bar{d}}Z_{e\bar{f}g\bar{h}}$. The use of barred indices is convenient for keeping track of which indices transform with U and which transform with $U^\dagger$. We also introduce the U(2)-invariant tensor $\delta_{a\bar{b}}$, which can be used to contract indices. In this notation, one can only contract an unbarred index against a barred index. For example,

$$Z^{(1)}_{a\bar{d}} \equiv \delta_{b\bar{c}}Z_{a\bar{b}c\bar{d}} = Z_{a\bar{b}b\bar{d}}, \qquad Z^{(2)}_{c\bar{d}} \equiv \delta_{b\bar{a}}Z_{a\bar{b}c\bar{d}} = Z_{a\bar{a}c\bar{d}}. \tag{19}$$

With respect to the Φ-basis of the unprimed scalar fields, we have

$$\begin{aligned} Y_{11} &= m^2_{11}, & Y_{12} &= -m^2_{12}, \\ Y_{21} &= -(m^2_{12})^*, & Y_{22} &= m^2_{22}, \end{aligned} \tag{20}$$

and

$$\begin{aligned} Z_{1111} &= \lambda_1, & Z_{2222} &= \lambda_2, \\ Z_{1122} &= Z_{2211} = \lambda_3, & Z_{1221} &= Z_{2112} = \lambda_4, \\ Z_{1212} &= \lambda_5, & Z_{2121} &= \lambda^*_5, \\ Z_{1112} &= Z_{1211} = \lambda_6, & Z_{1121} &= Z_{2111} = \lambda^*_6, \\ Z_{2212} &= Z_{1222} = \lambda_7, & Z_{2221} &= Z_{2122} = \lambda^*_7. \end{aligned} \tag{21}$$

For ease of notation, we have omitted the bars from the barred indices in Eqs. (20) and (21). Since the tensors $Y_{a\bar{b}}$ and $Z_{a\bar{b}c\bar{d}}$ exhibit tensorial properties with respect to global U(2) rotations in the Higgs flavor space, one can easily construct invariants with respect to the U(2) by forming U(2)-scalar quantities.

In Sec. III, we shall argue that the scalar potential is *CP* conserving if and only if a real basis exists. In this case, *all* possible U(2)-invariant scalars are manifestly real. Conversely, if the scalar potential explicitly violates *CP*, then there must exist at least one manifestly complex U(2)-scalar invariant. We shall exhibit the simplest set of independent potentially complex U(2)-scalar invariants that can be employed to test for explicit *CP* invariance or noninvariance of the 2HDM scalar potential.

III. COMPLEX INVARIANTS AND THE CONDITIONS FOR A *CP*-CONSERVING 2HDM SCALAR POTENTIAL

Given an arbitrary 2HDM Higgs potential, we have already noted that the scalar potential possesses a number of potentially complex parameters. We would like to determine in general whether this scalar potential is explicitly *CP* violating or *CP* conserving. The answer to this question is governed by a simple theorem:

Theorem 1.—The Higgs potential is explicitly *CP* conserving if and only if a basis exists in which all Higgs potential parameters are real. Otherwise, *CP* is explicitly violated.

Although Theorem 1 is well known and often stated in the literature, its proof is usually given under the assumption that a convenient basis has been chosen in which the *CP* transformation laws of the scalar fields assume a particularly simple form [4]. In Appendix A, we provide a general proof of Theorem 1 that does not make any assumption about the initial choice of the scalar field basis. As already noted, it may be difficult to determine whether a basis exists in which all Higgs potential parameters are real. Thus, we would like to reformulate Theorem 1 in a basis-independent language. That is, we propose to express the conditions for an explicitly *CP*-violating (or conserving) Higgs potential in terms of basis-independent invariants.

Before presenting the basis-independent version of Theorem 1, let us first enumerate the number of independent *CP*-violating phases that exist among the scalar potential parameters of the 2HDM. In Eq. (1), we have noted four potentially complex parameters: $Y_{12} \equiv -m_{12}^2$, λ_5, λ_6 and λ_7. Naively, it appears that there are three independent *CP*-violating phases, since one can always perform a phase rotation on one of the Higgs fields to render one of the complex parameters real. However, this conclusion is not correct, since one can utilize a larger SU(2) global symmetry to absorb additional phases.[4] An SU(2) global rotation is parametrized by one angle and two phases. This can be used to remove one real parameter and two phases from the initial ten real parameters and four phases that make up the scalar potential parameters. Thus, ultimately, the number of physical parameters of the scalar potential must be given by nine real parameters and two phases. Equivalently, there can only be two independent complex parameters among the physical parameters that describe the scalar potential.

This result can be derived in a very simple and direct fashion as follows [6]. Consider the explicit forms of $Z^{(1)}$ and $Z^{(2)}$ defined in Eq. (19):

$$Z^{(1)} = \begin{pmatrix} \lambda_1 + \lambda_4 & \lambda_6 + \lambda_7 \\ \lambda_6^* + \lambda_7^* & \lambda_2 + \lambda_4 \end{pmatrix}, \qquad Z^{(2)} = \begin{pmatrix} \lambda_1 + \lambda_3 & \lambda_6 + \lambda_7 \\ \lambda_6^* + \lambda_7^* & \lambda_2 + \lambda_3 \end{pmatrix}. \tag{22}$$

Note that $Z^{(1)}$ and $Z^{(2)}$ are Hermitian matrices that commute so that they can be simultaneously diagonalized by a unitary matrix. It therefore follows that there exists a basis in which $Z^{(1)}$ and $Z^{(2)}$ are simultaneously diagonal; that is, $\lambda_7 = -\lambda_6$. Once this basis is established, it is clear that the phase of λ_6 and λ_7 can be removed by a U(1) phase rotation of Φ_2. Thus, a basis can always be found in which only two parameters Y_{12} and λ_5 are complex. Moreover, the total number of independent real parameters is nine (since in a basis where $\lambda_7 = -\lambda_6$, only one of these two parameters is an independent degree of freedom). This matches the counting of parameters given in the previous paragraph.

Based on this parameter counting, one is tempted to conclude that there should be only two independent potentially complex invariants. Nevertheless, this intuition is misleading. The correct statement is summarized by the following theorem.

Theorem 2.—The necessary and sufficient conditions for an explicitly *CP*-conserving 2HDM scalar potential consist of the (simultaneous) vanishing of the imaginary parts of four potentially complex invariants:

$$I_{Y3Z} \equiv \mathrm{Im}(Z^{(1)}_{a\bar{c}} Z^{(1)}_{e\bar{b}} Z_{b\bar{e}c\bar{d}} Y_{d\bar{a}}), \tag{23}$$

$$I_{2Y2Z} \equiv \mathrm{Im}(Y_{a\bar{b}} Y_{c\bar{d}} Z_{b\bar{a}d\bar{f}} Z^{(1)}_{f\bar{c}}), \tag{24}$$

$$I_{6Z} \equiv \mathrm{Im}(Z_{a\bar{b}c\bar{d}} Z^{(1)}_{b\bar{f}} Z^{(1)}_{d\bar{h}} Z_{f\bar{a}j\bar{k}} Z_{k\bar{j}m\bar{n}} Z_{n\bar{m}h\bar{c}}), \tag{25}$$

$$I_{3Y3Z} \equiv \mathrm{Im}(Z_{a\bar{c}b\bar{d}} Z_{c\bar{e}d\bar{g}} Z_{e\bar{h}f\bar{q}} Y_{g\bar{a}} Y_{h\bar{b}} Y_{q\bar{f}}). \tag{26}$$

Henceforth, the imaginary parts of potentially complex invariants shall be referred to as *I-invariants*.

The case of $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ is a special isolated point in the scalar potential parameter space. In particular, when $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$, the matrices $Z^{(1)}$ and $Z^{(2)}$ are both proportional to the unit matrix. Thus, if both equalities $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ are true in one basis, then they must also be true in *all* bases [as previously noted below Eq. (8)]. Thus, Theorem 2 breaks up into two distinct cases:

[4] As previously noted, a U(1) hypercharge global rotation leaves all the scalar parameters unchanged; that is, the angle ψ in Eq. (4) has no effect. If one chooses $\psi = \frac{1}{2}(\xi - \chi)$, then the matrix U given in Eq. (4) is an SU(2) matrix.

(i) For the isolated point $\lambda_1 = \lambda_2$ *and* $\lambda_7 = -\lambda_6$, $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = 0$ is automatic [see Eqs. (28)–(30)]. In this case, the necessary and sufficient condition for an explicitly *CP*-conserving 2HDM scalar potential is simply given by $I_{3Y3Z} = 0$.

(ii) Away from the special isolated point of case (i), only three of the *I*-invariants need be considered. Specifically, at *any* other point of the parameter space, the necessary and sufficient conditions for an explicitly *CP*-conserving 2HDM scalar potential are given by[5]

$$I_{Y3Z} = I_{2Y2Z} = I_{6Z} = 0. \qquad (27)$$

It is trivial to prove that the above conditions are necessary for explicit *CP* conservation. If any of the above *I*-invariants [Eqs. (23)–(26)] are nonzero, then we can immediately conclude that no basis exists in which all scalar potential parameters are real. Thus, by Theorem 1, the scalar potential would be *CP* violating. The proof that the conditions of Theorem 2 are sufficient for explicit *CP* conservation will now be given, with further details provided in Appendixes C and D.

First, we must prove that all four *I*-invariants listed in Eqs. (23)–(26) are required in the formulation of Theorem 2. This may be accomplished by exhibiting four different models in which only one of the four *I*-invariants is nonzero. In Secs. IV A and IV C, we give explicit forms for these four *I*-invariants in a generic basis [see Eqs. (39), (41), (47), and (48), respectively]. However, as already noted below Eq. (22), it is always possible to choose a basis in which $\lambda_7 = -\lambda_6$. This basis is not unique, since further basis transformations can be performed while maintaining $\lambda_7 = -\lambda_6$. In any such basis, three of the *I*-invariants take particularly simple forms:

$$I_{Y3Z} = -(\lambda_1 - \lambda_2)^2 \mathrm{Im}(Y_{12}\lambda_6^*), \qquad (28)$$

$$I_{2Y2Z} = (\lambda_1 - \lambda_2)[\mathrm{Im}(Y_{12}^2\lambda_5^*) + (Y_{11} - Y_{22})\mathrm{Im}(Y_{12}\lambda_6^*)], \qquad (29)$$

$$I_{6Z} = -(\lambda_1 - \lambda_2)^3 \mathrm{Im}(\lambda_6^2\lambda_5^*). \qquad (30)$$

The expression for I_{3Y3Z} in this basis is more complicated:

$$\begin{aligned} I_{3Y3Z} = {} & 2\mathrm{Im}(Y_{12}^3\lambda_6(\lambda_5^*)^2) - 4\mathrm{Im}(Y_{12}^3(\lambda_6^*)^3) + [(Y_{11} - Y_{22})^2 - 6|Y_{12}|^2](Y_{11} - Y_{22})\mathrm{Im}(\lambda_6^2\lambda_5^*) \\ & + [(\lambda_1 - \lambda_3 - \lambda_4)(\lambda_2 - \lambda_3 - \lambda_4) + 2|\lambda_6|^2 - |\lambda_5|^2](Y_{11} - Y_{22})\mathrm{Im}(Y_{12}^2\lambda_5^*) \\ & + \{(\lambda_1 - \lambda_2)^2 Y_{11}Y_{22} + (4|\lambda_6|^2 - 2|\lambda_5|^2)[(Y_{11} - Y_{22})^2 - |Y_{12}|^2]\}\mathrm{Im}(Y_{12}\lambda_6^*) \\ & - (\lambda_1 + \lambda_2 - 2\lambda_3 - 2\lambda_4)\{(Y_{11} - Y_{22})\mathrm{Im}(Y_{12}^2(\lambda_6^*)^2) - \mathrm{Im}(Y_{12}^3\lambda_5^*\lambda_6^*) + [(Y_{11} - Y_{22})^2 - |Y_{12}|^2]\mathrm{Im}(Y_{12}\lambda_6\lambda_5^*)\}. \end{aligned} \qquad (31)$$

Working in the $\lambda_7 = -\lambda_6$ basis, we consider the four models:

(1) $Y_{a\bar{b}} = 0$ and $\lambda_1 \neq \lambda_2$;
(2) $\lambda_6 = 0$, $\lambda_1 \neq \lambda_2$ and $Y_{11} = Y_{22}$;
(3) $\lambda_5 = 0$, $\lambda_1 \neq \lambda_2$, $Y_{11} = Y_{22} = 0$ and $\mathrm{Re}(Y_{12}\lambda_6^*) = 0$;
(4) $\lambda_1 = \lambda_2$.

Then, in model 1, $I_{Y3Z} = I_{2Y2Z} = I_{3Y3Z} = 0$ whereas I_{6Z} is potentially nonzero. In model 2, $I_{Y3Z} = I_{6Z} = I_{3Y3Z} = 0$ whereas I_{2Y2Z} is potentially nonzero. In model 3, $I_{2Y2Z} = I_{6Z} = I_{3Y3Z} = 0$ whereas I_{Y3Z} is potentially nonzero.[6] Finally, in model 4, $I_{Y3Z} = I_{6Z} = I_{2Y2Z} = 0$ whereas I_{3Y3Z} is potentially nonzero. Thus, we have exhibited four separate models in which *CP* can be violated explicitly, and in each case only one of the four *I*-invariants is nonzero. This illustrates that all four *I*-invariants are needed to test whether the Higgs potential explicitly conserves or violates *CP*.

The requirement of four *I*-invariants in the formulation of Theorem 2 seems to be in conflict with our previous observation that the number of physical parameters of the 2HDM includes only *two* phases [see discussion surrounding Eq. (22)]. However, one can show that for any particular model, at most two *I*-invariants need be considered. To verify this assertion, we first transform to a basis in which $\lambda_7 = -\lambda_6$ and where λ_6 (and therefore λ_7) are real.[7] Then there are a number of cases to consider. (i) If $\lambda_1 = \lambda_2$, then $I_{3Y3Z} = 0$ implies that the Higgs sector is explicitly *CP* conserving. (ii) If $\lambda_1 \neq \lambda_2$ and Y_{12}, λ_5 and λ_6 are nonvanishing, then $I_{Y3Z} = I_{6Z} = 0$ implies that the Higgs sector is explicitly *CP* conserving. (iii) If $\lambda_1 \neq \lambda_2$ and two of the quantities Y_{12}, λ_5 and λ_6 are nonzero while the third vanishes, then only one *I*-invariant need be considered. Specifically, for $\lambda_5 = 0$ [$\lambda_6 = 0$], $I_{Y3Z} = 0$ [$I_{2Y2Z} = 0$] guarantees a *CP*-conserving Higgs sector, whereas for $Y_{12} = 0$, $I_{6Z} = 0$ guarantees a *CP*-conserving Higgs sector. Thus, we have shown that it is sufficient to examine at most two *I*-invariants to determine whether all four *I*-invariants [Eqs. (23)–(26)] simultaneously vanish.[8]

To complete the proof of Theorem 2, we must show that if the four *I*-invariants given by Eqs. (23)–(26) vanish, then

[5]If Eq. (27) is satisfied in case (ii), then $I_{3Y3Z} = 0$. Thus, the latter is not needed as a separate requirement.

[6]Note that if $\lambda_5 = 0$ and $Y_{11} = Y_{22}$, then Eq. (31) yields $I_{3Y3Z} = \{(\lambda_1 - \lambda_2)^2 Y_{11}Y_{22} - 16[\mathrm{Re}(Y_{12}\lambda_6^*)]^2\}\mathrm{Im}(Y_{12}\lambda_6^*)$.

[7]This is always possible as shown below Eq. (22).

[8]Of course, to take advantage of this observation in practice, one must be able to take the original model and transform to a basis where $\lambda_7 = -\lambda_6$ is real. In general, this may be difficult (and require a numerical computation). Thus, in order to test for explicit *CP* violation, it is often simpler to directly evaluate all four *I*-invariants in the original basis.

one can find a basis where all Higgs potential parameters are real. The proof is most easily carried out by first transforming to a basis in which $\lambda_7 = -\lambda_6$ and where λ_6 (and therefore λ_7) are real. In this basis, the two cases of $\lambda_1 = \lambda_2$ and $\lambda_1 \neq \lambda_2$ must be treated separately. First, we consider the case where $\lambda_1 \neq \lambda_2$. If $\lambda_7 = -\lambda_6 \neq 0$, then $I_{6Z} = 0$ [Eq. (30)] implies that λ_5 is also real in this basis, and $I_{Y3Z} = 0$ [Eq. (28)] implies that Y_{12} is real. We have therefore achieved a basis in which all scalar potential parameters are real. If $\lambda_6 = \lambda_7 = 0$, then one can perform a phase rotation on one of the scalar fields so that λ_5 is real, with Y_{12} potentially complex. In this new basis, if $\lambda_5 \neq 0$ then $I_{2Y2Z} = 0$ implies that Y_{12} is either real or purely imaginary. In the latter case, Eqs. (12)–(14) demonstrate that a U(2) transformation [see Eq. (4)] with parameters $\xi = \pi/2$, $\sin 2\theta = 0$ and $\chi = 0$ yields a basis in which $\lambda'_6 = -\lambda'_7 = 0$, and both $\lambda'_5 = -\lambda_5$ and Y'_{12} are real. Finally, if $\lambda_5 = \lambda_6 = \lambda_7 = 0$, then one can absorb any phase of Y_{12} into a phase redefinition of one of the scalar fields.

Next, we consider the case where $\lambda_1 = \lambda_2$ in a basis where $\lambda_7 = -\lambda_6$. In this case, it is always possible to make a further change of basis so that λ_5, λ_6 and λ_7 are real (this assertion is Lemma 2, which is proved in Appendix C).[9] In this latter basis where Y_{12} is potentially complex but all other scalar potential parameters are real, Eq. (31) yields the following form for the only potentially nonvanishing invariant I_{3Y3Z}:

$$\begin{aligned} I_{3Y3Z} = {} & 2\,\mathrm{Im}Y_{12}[\lambda_5^2 + \lambda_5(\lambda_1 - \lambda_3 - \lambda_4) - 2\lambda_6^2] \\ & \times [4\lambda_6(\mathrm{Re}Y_{12})^2 - \lambda_6(Y_{11} - Y_{22})^2 \\ & - (\lambda_3 + \lambda_4 + \lambda_5 - \lambda_1)(Y_{11} - Y_{22})\mathrm{Re}Y_{12}]. \end{aligned} \tag{32}$$

Then, $I_{3Y3Z} = 0$ implies that one of the following three conditions must be true in a basis where all the λ_i are real: (i) Y_{12} is real; (ii) $\lambda_5^2 + \lambda_5(\lambda_1 - \lambda_3 - \lambda_4) - 2\lambda_6^2 = 0$; or (iii) $4\lambda_6(\mathrm{Re}Y_{12})^2 - (\lambda_3 + \lambda_4 + \lambda_5 - \lambda_1)(Y_{11} - Y_{22})\mathrm{Re}Y_{12} - \lambda_6(Y_{11} - Y_{22})^2 = 0$. In Appendix D, we prove Lemma 4 which demonstrates that if Y_{12} is complex and either condition (ii) or condition (iii) holds, then it is possible to find a basis in which Y_{12} is real, while maintaining the reality of λ_5, λ_6 and λ_7. Hence it follows that if $I_{3Y3Z} = 0$, then there exists a basis in which all 2HDM scalar potential parameters are real.[10] The proof of Theorem 2 is now complete.

It is instructive to compare the results of Theorem 2 to one of the basis-dependent conditions that has been proposed in the literature. In a generic basis, a sufficient set of conditions for an explicitly CP-conserving 2HDM scalar potential is

$$\begin{aligned} \mathrm{Im}(Y_{12}^2\lambda_5^*) &= \mathrm{Im}(Y_{12}\lambda_6^*) = \mathrm{Im}(Y_{12}\lambda_7^*) = \mathrm{Im}(\lambda_5^*\lambda_6^2) \\ &= \mathrm{Im}(\lambda_5^*\lambda_7^2) = \mathrm{Im}(\lambda_6^*\lambda_7) = 0, \end{aligned} \tag{33}$$

where $Y_{12} \equiv -m_{12}^2$. Clearly, if Eq. (33) is satisfied, then a simple phase rotation of one of the scalar fields easily produces a basis in which all the scalar potential parameters are real. However, Eq. (33) is not necessary for CP conservation. In particular, the following statement is generally false: "the Higgs potential is explicitly CP violating if one or more of the quantities listed in Eq. (33) are nonvanishing." This is most easily demonstrated by the following exercise. Start with a model in which all potentially complex scalar potential parameters are real. Then, change the basis with a generic U(2) transformation [Eq. (4)]. In a typical case, the resulting parameters Y'_{12}, λ'_5, λ'_6, and λ'_7 in the new basis are complex, and one or more of the quantities listed in Eq. (33) are nonvanishing. Thus, Eq. (33) is not a necessary condition for an explicitly CP-conserving Higgs potential.[11]

Despite the relative simplicity of the forms for I_{Y3Z}, I_{2Y2Z}, I_{6Z} and I_{3Y3Z} in the $\lambda_7 = -\lambda_6$ basis, realistic models rarely conform to this particular basis choice. The power of the basis-independent formulation of Theorem 2 thus becomes evident when considering models where the transformation from the generic basis to the $\lambda_7 = -\lambda_6$ basis is not particularly simple. Fortunately, we possess expressions for these I-invariants in a generic basis [see Eqs. (39), (41), (47), and (48)], so there is no compelling need to explicitly perform this change of basis. For purposes of illustration, let us consider three special models. In model (i),

$$\lambda_1 = \lambda_2, \qquad \lambda_6 = \lambda_7 \quad \text{and} \quad Y_{11} = Y_{22}, \tag{34}$$

where Y_{12}, λ_5 and λ_6 have arbitrary phases. In model (ii),

$$\lambda_1 + \lambda_2 = 2(\lambda_3 + \lambda_4), \quad \lambda_5 = 0 \quad \text{and} \quad \lambda_6 = \lambda_7, \tag{35}$$

where Y_{12} and λ_6 have arbitrary phases. In model (iii),

$$\begin{aligned} &\lambda_1 = \lambda_2, \qquad \lambda_6 = \lambda_7^*, \\ &Y_{11} = Y_{22} \quad \text{and} \quad Y_{12}, \lambda_5 \text{ real}, \end{aligned} \tag{36}$$

where λ_6 has an arbitrary phase. Model (iii) arises by imposing on the Higgs potential a discrete permutation symmetry that interchanges Φ_1 and Φ_2 [14].

In the three models above, we have used Eqs. (39), (41), (47), and (48) in the generic basis to verify that $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = I_{3Y3Z} = 0$. Thus models (i), (ii) and (iii) are explicitly CP conserving. These three models also provide examples of explicitly CP-conserving 2HDM potentials

[9] In Appendix C, Lemma 3 demonstrates why the condition of $\lambda_1 = \lambda_2$ is crucial to the proof of Lemma 2.

[10] The U(2) rotation required to go to this basis is explicitly constructed in Appendix D.

[11] An example that illustrates the same point is a model in which $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$. Lemma 2 of Appendix C implies that we can transform to a basis in which all the λ_i are real. Nevertheless, in this basis, Eq. (32) implies that it is possible to have an explicitly CP-conserving model with $I_{3Y3Z} = 0$ and $\mathrm{Im}Y_{12} \neq 0$.

where Eq. (33) is *not* satisfied. Nevertheless, having verified that all the I-invariants vanish, one is assured of the existence of some basis choice for each model for which all Higgs potential parameters are real.

Here, we provide one explicit example in the case of model (iii). Starting from the generic basis specified in Eq. (36), we perform a U(2) transformation [Eq. (4)] with $\theta = \pi/4$ and $\xi = 0$. Then, Eqs. (7), (13), and (14) yield $m_{12}^{\prime 2} = \lambda_6' = \lambda_7' = 0$, while Eq. (12) implies that

$$\lambda_5' e^{2i\chi} = \frac{1}{2}(\lambda_1 - \lambda_3 - \lambda_4 + \lambda_5) - 2i\,\mathrm{Im}\lambda_6. \qquad (37)$$

It is now a simple matter to adjust χ so that λ_5' is real. Thus, we have exhibited the U(2) transformation that produces the real basis of model (iii) in which all scalar potential parameters are real. Applying this U(2) transformation to the fields, it is easy to check that the resulting real basis exhibits a discrete symmetry $\Phi_1' \to \Phi_1'$, $\Phi_2' \to -\Phi_2'$. Models that respect the latter discrete symmetry are manifestly *CP* invariant since λ_5' is the only potentially complex parameter, whose phase can be rotated away by an appropriate phase rotation of $\Phi_2' \to e^{i\eta}\Phi_2'$.

IV. A SURVEY OF COMPLEX INVARIANTS

In general, it is possible to construct an nth-order invariant quantity for any integer value of n, where n is the total number of Y's and Z's that appears in the invariant. The vast majority of such invariants are manifestly real. In this section, we focus on those invariants that are potentially complex.

The necessary and sufficient conditions for *CP* conservation have been presented in Theorem 2 and depend on only four potentially complex invariants given by Eqs. (23)–(26). However, new potentially complex nth-order invariants arise at every order (for $n > 4$) that cannot be expressed in terms of lower-order invariants. Nevertheless, Theorem 2 guarantees that if the I-invariants of Eqs. (23)–(26) vanish, then the imaginary parts of *all* potentially complex invariants must vanish. In particular, we have explicitly verified the following statements:

(1) All invariants (of arbitrary order) that are either independent of Z or linear in Z are manifestly real.
(2) All invariants of cubic order or less are manifestly real.
(3) Any quartic (i.e., fourth-order) I-invariant is a real linear combination of I_{Y3Z} and I_{2Y2Z}.
(4) Any fourth- or higher-order I-invariant that is quadratic in Z is proportional to I_{2Y2Z}.
(5) Any fifth-order I-invariant vanishes if $I_{Y3Z} = I_{2Y2Z} = 0$.
(6) Any sixth-order I-invariant that is independent of Y is proportional to I_{6Z}. Moreover, if $Y_{a\bar{b}} = 0$ then any I-invariant of arbitrary order vanishes if $I_{6Z} = 0$.
(7) Any sixth-order I-invariant that is both cubic in Y and Z respectively is a real linear combination of I_{3Y3Z} and lower-order invariants that vanish if $I_{Y3Z} = I_{2Y2Z} = 0$.
(8) Any sixth-order I-invariant that is either linear or quadratic in Y vanishes if $I_{Y3Z} = I_{2Y2Z} = 0$.

Finally, we reiterate that

(9) Any I-invariant of arbitrary order vanishes if $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = I_{3Y3Z} = 0$.

This last result is a consequence of Theorem 2. The explicit verification of statements 1–8 is based on a systematic study of potentially complex U(2)-invariant scalars made up of the tensors $Y_{a\bar{b}}$ and $Z_{a\bar{b}c\bar{d}}$. This study gives us further confidence that the ultimate conclusion given by statement (9) above is correct.

We begin this study by noting that for $n = 1$, the only invariants are $\mathrm{Tr}Y$, $\mathrm{Tr}Z^{(1)}$ and $\mathrm{Tr}Z^{(2)}$, all of which are manifestly real. For $n = 2$, the possible quadratic invariants include the products of the first order invariants and $\mathrm{Tr}(Y^2)$, $\mathrm{Tr}(YZ^{(1)})$, $\mathrm{Tr}(YZ^{(2)})$, $\mathrm{Tr}(Z^{(i)}Z^{(j)})$ [for $i, j = 1, 2$], $\mathrm{Tr}Z^{(31)} \equiv Z_{a\bar{b}c\bar{d}}Z_{b\bar{a}d\bar{c}}$ and $\mathrm{Tr}Z^{(32)} \equiv Z_{a\bar{b}c\bar{d}}Z_{d\bar{a}b\bar{c}}$, where $Z^{(31)}$ and $Z^{(32)}$ are introduced in Eq. (E3).[12] By inspection, all such quadratic invariants are manifestly real. Turning to the cubic invariants, the enumeration of all possible cases becomes significantly more complex. Nevertheless, it is still possible to show by hand that all cubic invariants are manifestly real. This is demonstrated in Appendix E. Thus, in order to find a potentially complex invariant, one must examine invariants of fourth order and higher. At this point, an explicit hand calculation quickly becomes infeasible, and we must employ a computer algebra program such as MATHEMATICA to assist in the analysis. For example, consider all possible invariants that are independent of $Y_{a\bar{b}}$ (such invariants will be called Z-invariants). One can use MATHEMATICA to evaluate the imaginary part of each invariant by explicitly considering invariants which consist of n-fold products of Z's. These invariants are of the form:

$$Z_{a_1\bar{b}_1c_1\bar{d}_1}Z_{a_2\bar{b}_2c_2\bar{d}_2}\cdots Z_{a_n\bar{b}_nc_n\bar{d}_n}, \qquad (38)$$

where one chooses the indices $\{b_1, d_1, b_2, d_2, \ldots, b_n, d_n\}$ to be a particular permutation of $\{a_1, c_1, a_2, c_2, \ldots, a_n, c_n\}$, and then sums over the repeated indices as usual. By considering all possible permutations, one generates all $(2n)!$ possible invariants (many of which are trivially related to others in the complete list of invariants). One can automate the computation with a MATHEMATICA program and compute the imaginary part of all $(2n)!$ invariants subject to the constraints of computer time. The procedure can be generalized to include some number of $Y_{a\bar{b}}$. In particular, it is easy to show (without computer assistance)

[12] The determinants of Y, $Z^{(1)}$ and $Z^{(2)}$ are quadratic invariants that are related to the invariants given above via the identity $\det M \equiv \frac{1}{2}[(\mathrm{Tr}M)^2 - \mathrm{Tr}(M^2)]$, which is satisfied by any 2×2 matrix.

that all invariants that are independent of Z (such invariants will be called Y-invariants) are manifestly real, due to the Hermiticity property of $Y_{a\bar{b}}$.

A. Fourth-order potentially complex invariants

Among the quartic invariants, we first construct all possible quartic Z-invariants. By an explicit MATHEMATICA computation, we were able to show that all $8! = 40\,320$ quartic Z-invariants are manifestly real.

We next search for potentially complex quartic invariants that are linear in Y. We display one potentially nonzero I-invariant below:

$$\begin{aligned} I_{Y3Z} \equiv\ & \mathrm{Im}(Z^{(1)}_{a\bar{c}} Z^{(1)}_{e\bar{b}} Z_{b\bar{e}c\bar{d}} Y_{d\bar{a}}) \\ =\ & 2(|\lambda_6|^2 - |\lambda_7|^2)\mathrm{Im}[Y_{12}(\lambda_6^* + \lambda_7^*)] \\ & + (\lambda_1 - \lambda_2)[\mathrm{Im}(Y_{12}\Lambda^*) - \mathrm{Im}[Y_{12}\lambda_5^*(\lambda_6 + \lambda_7)]] \\ & + (Y_{11} - Y_{22})[\mathrm{Im}[\lambda_5^*(\lambda_6 + \lambda_7)^2] \\ & - (\lambda_1 - \lambda_2)\mathrm{Im}(\lambda_7^*\lambda_6)], \end{aligned} \tag{39}$$

where

$$\Lambda \equiv (\lambda_2 - \lambda_3 - \lambda_4)\lambda_6 + (\lambda_1 - \lambda_3 - \lambda_4)\lambda_7. \tag{40}$$

Using MATHEMATICA, we have evaluated the imaginary part of all $7! = 5040$ possible invariants that are linear in Y and cubic in Z. We find that the result either vanishes or is equal to $\pm I_{Y3Z}$.

Next, we examine potentially complex quartic invariants that are quadratic in both Y and Z. We display one potentially nonzero I-invariant in Eq. (41):

$$\begin{aligned} I_{2Y2Z} \equiv\ & \mathrm{Im}(Y_{a\bar{b}} Y_{c\bar{d}} Z_{b\bar{a}d\bar{f}} Z^{(1)}_{f\bar{c}}) \\ =\ & (\lambda_1 - \lambda_2)\mathrm{Im}(Y_{12}^2\lambda_5^*) \\ & - (Y_{11} - Y_{22})[\mathrm{Im}(Y_{12}\Lambda^*) + \mathrm{Im}(Y_{12}\lambda_5^*(\lambda_6 + \lambda_7))] \\ & - \mathrm{Im}[(Y_{12}\lambda_6^*)^2] + \mathrm{Im}[(Y_{12}\lambda_7^*)^2] \\ & + [(Y_{11} - Y_{22})^2 - 2|Y_{12}|^2]\mathrm{Im}(\lambda_7^*\lambda_6). \end{aligned} \tag{41}$$

Moreover, we find as before that the imaginary parts of all such invariants (there are $6! = 720$ invariants that are quadratic in both Y and Z) either vanish or are equal to $\pm I_{2Y2Z}$.

It is easy to show that quartic invariants that are cubic in Y (and therefore linear in Z) are manifestly real. In particular, there are only two such invariants that are not a product of lower-order invariants: $\mathrm{Tr}(Y^3 Z^{(1)})$ and $\mathrm{Tr}(Y^3 Z^{(2)})$. Both these invariants are manifestly real due to the Hermiticity properties of Y, $Z^{(1)}$ and $Z^{(2)}$.

B. Fifth-order potentially complex invariants

We begin by constructing all possible fifth-order Z-invariants. Again, with the help of MATHEMATICA, we found that all $10! = 3\,628\,800$ Z-invariants are manifestly real. Next, we considered the $Y4Z$ invariants, i.e. the fifth-order invariants that are linear in Y. After computing the imaginary parts of all $9! = 362\,880$ such invariants, we found that only one genuinely new potentially complex invariant emerged. The corresponding I-invariant is

$$\begin{aligned} I_{Y4Z} =\ & \mathrm{Im}[Z^{(2)}_{a\bar{b}} Z_{b\bar{a}c\bar{d}} Z^{(2)}_{d\bar{e}} Z_{e\bar{c}f\bar{g}} Y_{g\bar{f}}] \\ =\ & -\lambda_4 I_{Y3Z} + (\lambda_1 - \lambda_2)\mathrm{Im}[Y_{12}(\lambda_6^* + \lambda_7^*)^2(\lambda_6^* - \lambda_7^*)] + \mathrm{Im}[Y_{12}\lambda_5^*(\lambda_6^2\lambda_7^* - \lambda_7^2\lambda_6^*)] + \mathrm{Im}[Y_{12}\lambda_5(\lambda_6^{*2} - \lambda_7^{*2})(\lambda_6^* + \lambda_7^*)] \\ & + \frac{1}{2}(-(\lambda_1 - \lambda_2)(\lambda_1 + \lambda_2 - 2\lambda_3 - 2\lambda_4) + |\lambda_7|^2 - |\lambda_6|^2)\mathrm{Im}[Y_{12}\lambda_5^*(\lambda_6 + \lambda_7)] \\ & - \frac{1}{2}[(\lambda_1 - \lambda_2)^2 - |\lambda_6|^2 - |\lambda_7|^2]\mathrm{Im}[Y_{12}\lambda_5^*(\lambda_6 - \lambda_7)] + \frac{1}{2}(\lambda_1 - \lambda_2)(2|\lambda_5|^2 - |\lambda_6|^2 - |\lambda_7|^2)\mathrm{Im}[Y_{12}(\lambda_6^* + \lambda_7^*)] \\ & + \frac{1}{2}(\lambda_1 - \lambda_2)(|\lambda_6|^2 - |\lambda_7|^2)\mathrm{Im}[Y_{12}(\lambda_6^* - \lambda_7^*)] + \frac{1}{2}(Y_{11} - Y_{22})\{4(|\lambda_6|^2 - |\lambda_7|^2)\mathrm{Im}(\lambda_6\lambda_7^*) + (\lambda_1 - \lambda_2)\mathrm{Im}[\lambda_5^*(\lambda_7^2 - \lambda_6^2)] \\ & + (\lambda_1 + \lambda_2 - 2\lambda_3 - 2\lambda_4)\mathrm{Im}[\lambda_5^*(\lambda_6 + \lambda_7)^2]\}, \end{aligned} \tag{42}$$

where I_{Y3Z} is given by Eq. (39). In addition, we have explicitly verified that the imaginary parts of all potentially complex $Y4Z$ invariants reduce to a linear combination of I_{Y4Z} and the product of I_{Y3Z} times a linear combination of $\mathrm{Tr}[Z^{(1)}]$ and $\mathrm{Tr}[Z^{(2)}]$.

The fact that I_{Y4Z} is a "new" I-invariant means that one cannot express I_{Y4Z} as a sum of terms, each of which is the imaginary part of a product of lower-order invariants. Nevertheless, one can show that if $I_{Y3Z} = I_{2Y2Z} = 0$, then it follows that $I_{Y4Z} = 0$. This is most easily accomplished in the basis where $\lambda_7 = -\lambda_6$. In this basis, Eq. (42) simplifies enormously:

$$I_{Y4Z} = (\lambda_1 - \lambda_2)^2[\lambda_4\mathrm{Im}(Y_{12}\lambda_6^*) - \mathrm{Im}(Y_{12}\lambda_6\lambda_5^*)]. \tag{43}$$

If $Y_{12} = 0$ in the $\lambda_7 = -\lambda_6$ basis then $I_{Y4Z} = 0$. Alternatively, if $Y_{12} \neq 0$, then we make use of

$$\begin{aligned} \mathrm{Im}\,(Y_{12}\lambda_6\lambda_5^*) =\ & \frac{1}{|Y_{12}|^2}[\mathrm{Im}(Y_{12}^2\lambda_5^*)\mathrm{Re}(Y_{12}\lambda_6^*) \\ & - \mathrm{Im}(Y_{12}\lambda_6^*)\mathrm{Re}(Y_{12}^2\lambda_5^*)]. \end{aligned} \tag{44}$$

Since $I_{Y3Z} = I_{2Y2Z} = 0$ implies that either $\lambda_1 = \lambda_2$ or $\mathrm{Im}(Y_{12}^2\lambda_5^*) = \mathrm{Im}(Y_{12}\lambda_6^*) = 0$ [see Eqs. (28) and (29)], one can again conclude that $I_{Y4Z} = 0$. Having proved that the *invariant* I_{Y4Z} vanishes in one basis, it immediately follows that $I_{Y4Z} = 0$ in *all* basis choices.

Similarly, we have analyzed the $2Y3Z$ invariants, i.e., the fifth-order invariants that are quadratic in Y and cubic in Z. Again, we have computed the imaginary parts of all 40 320 such invariants. We have explicitly verified that any potentially complex fifth-order invariant of this type is a linear combination of I_{Y3Z} (with coefficient proportional to $\mathrm{Tr}Y$), I_{2Y2Z} (with coefficient proportional to a linear combination of $\mathrm{Tr}[Z^{(1)}]$ and $\mathrm{Tr}[Z^{(2)}]$) and one new potentially complex invariant form. A particular choice for the new I-invariant is

$$I_{2Y3Z} = \mathrm{Im}[Z_{a\bar{c}b\bar{e}} Z_{c\bar{f}d\bar{b}} Z_{e\bar{g}f\bar{h}} Y_{g\bar{a}} Y_{h\bar{d}}]. \tag{45}$$

One could write out the explicit expression for I_{2Y3Z} [as we did in Eq. (42) for I_{Y4Z}]. However, for our purposes, it is sufficient to give the form of I_{2Y3Z} in the $\lambda_7 = -\lambda_6$ basis:

$$\begin{aligned} I_{2Y3Z} = {} & (\lambda_1 - \lambda_2)\{4\,\mathrm{Im}(Y_{12}^2 \lambda_6^{*2}) + 2(Y_{11} - Y_{22})\mathrm{Im}[Y_{12}\lambda_5^* \lambda_6] \\ & - (\lambda_1 + \lambda_2 - 2\lambda_3)\mathrm{Im}(Y_{12}^2 \lambda_5^*) - 2\lambda_4 (Y_{11} - Y_{22})\mathrm{Im}(Y_{12}\lambda_6^*)\}. \end{aligned} \tag{46}$$

Again, we emphasize that I_{2Y3Z} is a new I-invariant in the sense that one cannot express I_{2Y3Z} as a sum of terms, each of which is the imaginary part of a product of lower-order invariants. Nevertheless, $I_{Y3Z} = I_{2Y2Z} = 0$ implies that $I_{2Y3Z} = 0$.[13]

The remaining cases are easily treated. We explicitly verified that any fifth-order invariants that are cubic in Y and quadratic in Z are proportional to $(\mathrm{Tr}Y) I_{2Y2Z}$. It is also simple to show that all fifth-order invariants that are linear in Z are manifestly real. In particular, the only two inequivalent invariants of this type that are not products of the lower-order invariants are $Z_{a\bar{b}c\bar{d}} Y_{b\bar{a}}^2 Y_{d\bar{c}}^2$ and $Z_{a\bar{b}c\bar{d}} Y_{b\bar{c}}^2 Y_{d\bar{a}}^2$. By explicit calculation, using the Hermiticity properties of Y and Z, it is straightforward to verify that both these invariants are real. We have previously noted that all pure Y-invariants are manifestly real. This completes the proof that all potentially complex fifth-order invariants are linear combinations of I_{Y3Z} and I_{2Y2Z} or forms that vanish when $I_{Y3Z} = I_{2Y2Z} = 0$. That is, the consideration of potentially complex fifth-order invariants does not establish any new independent conditions for CP violation.

C. Sixth-order potentially complex invariants

Two new independent conditions for CP violation arise from the study of sixth-order potentially complex invariants. We begin by constructing all possible sixth-order Z-invariants. It is here that we encounter the first potentially complex Z-invariants. One potentially nonzero I-invariant is

$$\begin{aligned} I_{6Z} \equiv {} & \mathrm{Im}(Z_{a\bar{b}c\bar{d}} Z^{(1)}_{b\bar{f}} Z^{(1)}_{d\bar{h}} Z_{f\bar{a}j\bar{k}} Z_{k\bar{j}m\bar{n}} Z_{n\bar{m}h\bar{c}}) \\ = {} & 2|\lambda_5|^2 \mathrm{Im}[(\lambda_7^* \lambda_6)^2] - \mathrm{Im}[\lambda_5^{*2}(\lambda_6 - \lambda_7)(\lambda_6 + \lambda_7)^3] + (\lambda_1 - \lambda_2)|\lambda_5|^2 \mathrm{Im}[\lambda_5^*(\lambda_6 + \lambda_7)^2] - (\lambda_1 - \lambda_2)\mathrm{Im}(\lambda_5^* \Lambda^2) \\ & + 2\mathrm{Im}(\lambda_7^* \lambda_6)[|\lambda_5|^2[|\lambda_6|^2 + |\lambda_7|^2 - (\lambda_1 - \lambda_2)^2] - 2(|\lambda_6|^2 - |\lambda_7|^2)^2] - 2(|\lambda_6|^2 - |\lambda_7|^2)\mathrm{Im}[\lambda_5^* \Lambda(\lambda_6 + \lambda_7)] \\ & + (\lambda_1 - \lambda_2)[\mathrm{Im}[\Lambda(\lambda_7 \lambda_6^{*2} + \lambda_6 \lambda_7^{*2} - |\lambda_7|^2 \lambda_6^* - |\lambda_6|^2 \lambda_7^*)] + 2\,\mathrm{Im}[\lambda_5((|\lambda_6|^2 + |\lambda_7|^2)\lambda_6^* \lambda_7^* - \lambda_7 \lambda_6^{*3} - \lambda_6 \lambda_7^{*3})]], \end{aligned} \tag{47}$$

where Λ is defined in Eq. (40).

Theorem 2 implies that if $Y_{a\bar{b}} = 0$ and $I_{6Z} = 0$, then any Z-invariant is real. Consequently, the imaginary part of any sixth-order Z-invariant must be equal to cI_{6Z}, for some real constant c. Our proof of Theorem 2 in Sec. III leaves no doubt as to the veracity of this conclusion. Nevertheless, it is instructive to check this assertion explicitly. Unfortunately, a complete survey of all possible $12! = 479\,001\,600$ sixth-order complex Z-invariants is beyond the capability of our desktop computers. However, we were able to examine roughly 9×10^6 sixth-order Z-invariants, and in these cases the imaginary part of each sixth-order Z-invariant either vanishes or is equal to $\pm I_{6Z}$ or $\pm 2I_{6Z}$.

If $\lambda_1 \neq \lambda_2$ in a basis where $\lambda_7 = -\lambda_6$, then Theorem 2 implies that $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = 0$ is a necessary and sufficient condition for an explicitly CP-conserving 2HDM scalar potential. However, the case of $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ (where $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = 0$ is automatic) must be treated separately. In this latter case, the condition for CP violation depends on an independent invariant that first arises at sixth order and is made up of three Y and three Z factors (henceforth denoted as $3Y3Z$ invariants).

Thus, we have constructed all possible $3Y3Z$ invariants and examined their imaginary parts. Of course, some of these will simply be linear combinations of lower-order invariants already examined. A complete survey of the imaginary part of all possible $9! = 362\,880$ $3Y3Z$ invariants yields one new independent I-invariant. A representative choice is

[13]This is easily verified after noting that $\mathrm{Im}(Y_{12}^2 \lambda_6^{*2}) = 2\,\mathrm{Im}(Y_{12}\lambda_6^*)\mathrm{Re}(Y_{12}\lambda_6^*)$.

$$
\begin{aligned}
I_{3Y3Z} &= \mathrm{Im}(Z_{a\bar{c}b\bar{d}}Z_{c\bar{e}d\bar{g}}Z_{e\bar{h}f\bar{q}}Y_{g\bar{a}}Y_{h\bar{b}}Y_{q\bar{f}}) \\
&= (Y_{11}-Y_{22})[(\lambda_1-\lambda_3-\lambda_4)(\lambda_2-\lambda_3-\lambda_4)-|\lambda_5|^2+|\lambda_6|^2+|\lambda_7|^2]\mathrm{Im}[Y_{12}^2\lambda_5^*]+\mathrm{Im}[Y_{12}^3\lambda_5^*\tilde{\Lambda}^*] \\
&\quad +2\,\mathrm{Im}[Y_{12}^3\lambda_6^*\lambda_7^*(\lambda_6^*-\lambda_7^*)]+[(Y_{11}-Y_{22})^2-|Y_{12}|^2]|\lambda_5|^2\mathrm{Im}[Y_{12}(\lambda_7^*-\lambda_6^*)]-Y_{11}Y_{22}(\lambda_1-\lambda_2)\mathrm{Im}[Y_{12}\Lambda^*] \\
&\quad +\mathrm{Im}[Y_{12}^3(\lambda_5^*)^2(\lambda_6-\lambda_7)]+2[(Y_{11}-Y_{22})^2+Y_{11}Y_{22}-|Y_{12}|^2][|\lambda_7|^2\mathrm{Im}(Y_{12}\lambda_6^*)-|\lambda_6|^2\mathrm{Im}(Y_{12}\lambda_7^*)] \\
&\quad -[(Y_{11}-Y_{22})^2-|Y_{12}|^2]\mathrm{Im}(Y_{12}\lambda_5^*\tilde{\Lambda})+2Y_{11}Y_{22}[|\lambda_7|^2\mathrm{Im}(Y_{12}\lambda_7^*)-|\lambda_6|^2\mathrm{Im}(Y_{12}\lambda_6^*)] \\
&\quad +(\lambda_1-\lambda_2)Y_{11}Y_{22}\mathrm{Im}[Y_{12}\lambda_5^*(\lambda_6+\lambda_7)]-(Y_{11}-Y_{22})\{(Y_{11}Y_{22}+|Y_{12}|^2)[\mathrm{Im}[\lambda_5^*(\lambda_6^2+\lambda_7^2)]-(\lambda_1-\lambda_2)\mathrm{Im}(\lambda_6\lambda_7^*)] \\
&\quad +(Y_{11}^2+Y_{22}^2-4|Y_{12}|^2)\mathrm{Im}[\lambda_5^*\lambda_6\lambda_7]-(\lambda_1+\lambda_2-2\lambda_3-2\lambda_4)\mathrm{Im}[Y_{12}^2\lambda_6^*\lambda_7^*]\}, \qquad (48)
\end{aligned}
$$

where Λ is defined in Eq. (40) and

$$\tilde{\Lambda} \equiv (\lambda_2-\lambda_3-\lambda_4)\lambda_6-(\lambda_1-\lambda_3-\lambda_4)\lambda_7. \qquad (49)$$

We have explicitly verified that the imaginary part of any $3Y3Z$ invariant is a real linear combination of I_{3Y3Z}, $(\mathrm{Tr}Y)I_{2Y3Z}$, $[\mathrm{Tr}Y]^2I_{Y3Z}$, $[\mathrm{Tr}Y^2]I_{Y3Z}$, $\mathrm{Tr}[YZ^{(1)}]I_{2Y2Z}$, $\mathrm{Tr}[YZ^{(2)}]I_{2Y2Z}$ and $(\mathrm{Tr}Y)(\mathrm{Tr}Z^{(1)})I_{2Y2Z}$.[14] In a basis where $\lambda_7=-\lambda_6$, I_{3Y3Z} reduces to the expression given by Eq. (31). Indeed, I_{3Y3Z} is nonzero in explicitly CP-violating models with $\lambda_7=-\lambda_6$ and $\lambda_1=\lambda_2$, which confirms that it is a necessary ingredient in the formulation of Theorem 2.

Among other sixth-order invariants, all $6Y$ and $Z5Y$ invariants are manifestly real. A $2Z4Y$ invariant is potentially complex, but its imaginary part must be proportional to some linear combination of $(\mathrm{Tr}Y)^2I_{2Y2Z}$ and $(\mathrm{Tr}Y^2)I_{2Y2Z}$. This leaves two interesting cases: the $Y5Z$ and $2Y4Z$ invariants, which we now consider in more detail.

A partial scan of the imaginary part of $10! = 3\,628\,800$ $2Y4Z$ invariants and $11! = 39\,916\,800$ $Y5Z$ invariants has been performed, and our results yield two genuinely new potentially complex invariants, whose imaginary parts we designate by I_{2Y4Z} and I_{Y5Z}, respectively. The resulting expressions in a generic basis are quite complicated and not very illuminating. Hence, here we provide only the explicit forms in a basis where $\lambda_7=-\lambda_6$:

$$
\begin{aligned}
I_{2Y4Z} &= \mathrm{Im}(Z^{(2)}_{b\bar{c}}Z_{c\bar{e}d\bar{f}}Z_{e\bar{q}f\bar{r}}Z_{g\bar{b}h\bar{d}}Y_{q\bar{g}}Y_{r\bar{h}}) \\
&= (\lambda_1-\lambda_2)\{(\lambda_1+\lambda_2)\mathrm{Im}(Y_{12}^2\lambda_6^{*2})-(\lambda_1\lambda_2-|\lambda_5|^2-2|\lambda_6|^2)\mathrm{Im}(Y_{12}^2\lambda_5^*) \\
&\quad +[2(\lambda_1Y_{11}-\lambda_2Y_{22})-(\lambda_3+\lambda_4)(Y_{11}-Y_{22})]\mathrm{Im}(Y_{12}\lambda_6\lambda_5^*) \\
&\quad +[2|\lambda_5|^2(Y_{11}-Y_{22})-(\lambda_3+\lambda_4)(\lambda_1Y_{11}-\lambda_2Y_{22})]\mathrm{Im}(Y_{12}\lambda_6^*)-[(Y_{11}-Y_{22})^2-2|Y_{12}|^2]\mathrm{Im}(\lambda_6^2\lambda_5^*)\}, \qquad (50)
\end{aligned}
$$

and

$$
\begin{aligned}
I_{Y5Z} &= \mathrm{Im}(Z^{(1)}_{b\bar{c}}Z_{c\bar{b}d\bar{e}}Z_{e\bar{d}f\bar{g}}Z^{(1)}_{g\bar{q}}Z_{q\bar{f}r\bar{s}}Y_{s\bar{r}}) \\
&= (\lambda_1-\lambda_2)^2\{(Y_{11}-Y_{22})\mathrm{Im}(\lambda_6^2\lambda_5^*) \\
&\quad +[\lambda_4(\lambda_1+\lambda_2)+\lambda_4^2-|\lambda_5|^2]\mathrm{Im}(Y_{12}\lambda_6^*) \\
&\quad -(\lambda_1+\lambda_2)\mathrm{Im}(Y_{12}\lambda_6\lambda_5^*)\}. \qquad (51)
\end{aligned}
$$

If $Y_{12}\neq 0$ in the $\lambda_7=-\lambda_6$ basis, then we can use

$$
\begin{aligned}
\mathrm{Im}\,(\lambda_6^2\lambda_5^*) &= \frac{1}{|Y_{12}|^2}[\mathrm{Re}(Y_{12}\lambda_6^*)\mathrm{Im}(Y_{12}\lambda_6\lambda_5^*) \\
&\quad -\mathrm{Re}(Y_{12}\lambda_6\lambda_5^*)\mathrm{Im}(Y_{12}\lambda_6^*)] \qquad (52)
\end{aligned}
$$

along with Eqs. (28), (29), and (44) to conclude that both I_{2Y4Z} and I_{Y5Z} vanish if $I_{Y3Z}=I_{2Y2Z}=0$.[15] However, if $Y_{12}=0$ in the $\lambda_7=-\lambda_6$ basis, then *all* invariants of nth-order with $n\leq 5$ are real. In the latter case, both I_{2Y4Z} and I_{Y5Z} can still be nonvanishing, which demonstrates that these are new I-invariants. Nevertheless, by the same argument as before, we may conclude that if $I_{Y3Z}=I_{2Y2Z}=I_{6Z}=0$, then both I_{2Y4Z} and I_{Y5Z} must vanish. For this reason, I_{2Y4Z} and I_{Y5Z} need not be independently considered in the formulation of Theorem 2.[16] In particular, I_{6Z} is included in the statement of Theorem 2, since (unlike I_{2Y4Z} and I_{Y5Z}) I_{6Z} can be nonzero even when $Y_{a\bar{b}}=0$.

We have verified[17] that the imaginary part of any $2Y4Z$ invariant can be expressed as a real linear combination of I_{2Y4Z}, I_{2Y3Z}, I_{2Y2Z} and I_{Y3Z}. Likewise, the imaginary part of any $Y5Z$ invariant can be expressed as a real linear combination of I_{Y5Z}, I_{Y4Z} and I_{Y3Z}. In both cases, each of the corresponding coefficients of the linear combination of terms are real invariant quantities. As an explicit illustra-

[14]Note that $\mathrm{Tr}Y\,\mathrm{Tr}Z^{(2)}=\mathrm{Tr}Y\,\mathrm{Tr}Z^{(1)}-\mathrm{Tr}[Y(Z^{(1)}-Z^{(2)})]$.

[15]Although this result is demonstrated in the $\lambda_7=-\lambda_6$ basis, the conclusion must hold for all basis choices.

[16]However, it is not possible to express either I_{2Y4Z} or I_{Y5Z} as a linear combination of I_{6Z}, I_{Y3Z} and I_{2Y2Z} with corresponding coefficients that are invariant quantities.

[17]Our conclusion is based on a partial scan of about 2×10^6 invariants. However, the arguments in the next subsection strongly suggest that the following results apply to all $2Y4Z$ and $Y5Z$ invariants.

tive example, we have verified

$$\begin{aligned}\mathrm{Im}[Z^{(2)}_{b\bar{c}} Z_{c\bar{b}d\bar{e}} Z_{e\bar{d}f\bar{g}} Z_{g\bar{q}h\bar{r}} Y_{q\bar{f}} Y_{r\bar{h}}] &= I_{2Y4Z} + \tfrac{1}{4}\mathrm{Tr}Z^{(1)} I_{2Y3Z} + \tfrac{1}{2}\mathrm{Tr}Y I_{Y4Z} \\ &\quad - \tfrac{1}{2}[\mathrm{Tr}(Z^{(1)}Z^{(2)}) - \tfrac{1}{2}(\mathrm{Tr}Z^{(1)})^2 + Z_{a\bar{c}b\bar{d}} Z_{c\bar{a}d\bar{b}}] I_{2Y2Z} \\ &\quad - \tfrac{1}{2}[\mathrm{Tr}(Z^{(1)}Y) + \tfrac{1}{2}\mathrm{Tr}Y\,\mathrm{Tr}Z^{(2)}] I_{Y3Z}. \end{aligned} \tag{53}$$

D. General results for *n*th-order potentially complex invariants

The analyses of Secs. IVA and IV B permit us to conjecture a number of results that we expect to hold for complex invariants of arbitrary order. These results provide a method for identifying the number of new potentially complex invariants at any order. As before, we define a new nth-order I-invariant to be one that cannot be written as a sum of terms, each of which is the imaginary part of a product of known invariants of order $\leq n$. By this definition, new I-invariants arise at each order (for $n \geq 4$). However, as previously stated, if $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = I_{3Y3Z} = 0$, then any new I-invariant that arises must also vanish.

Consider an arbitrary nth-order I-invariant I_{pYqZ} made up of p factors of Y and $q = n - p$ factors of Z. In a basis where $\lambda_7 = -\lambda_6$, for $p \leq 3$

$$I_{pYqZ} = (\lambda_1 - \lambda_2)^{3-p} \mathrm{Im} P(Y_{12}, \lambda_5, \lambda_6), \tag{54}$$

where P is a polynomial of its arguments and their complex conjugates constructed such that each term in the sum contains p factors of $Y_{a\bar{b}}$ and $q + p - 3$ factors of the λ_i, with the constraint that the weight of each term in the sum is zero. Here, we define the weight w according to the rules: $w(Y_{12}) = +1$, $w(\lambda_5) = +2$, $w(\lambda_6) = +1$, $w(x^*) = -w(x)$ for any x and $w(xy) = w(x) + w(y)$ for any x, y.[18]

The polynomial P possesses one additional property of note: it does not vanish in the limit of $\lambda_1 = \lambda_2$ (assuming that $P \neq 0$ in general). That is, the behavior of I_{pYqZ} in the $\lambda_1 \to \lambda_2$ limit is specified explicitly in Eq. (54). If $p > 3$, then $I_{pYqZ} = 0$. For example at sixth order, $\mathrm{Tr}(Y^2) I_{2Y2Z}$ is a potentially nonvanishing I-invariant with $p = 4$, but this does not constitute a new I-invariant by the above definition.

Equation (54) is consistent with all the results of Secs. IVA and IV B. It also provides an explanation for the absence of complex invariants of low order. For example, if we apply Eq. (54) and attempt to construct I_{5Z}, we would need to find a polynomial P with a nonzero imaginary part that is quadratic in the λ_i. No such polynomial exists, and we conclude that $I_{5Z} = 0$. We can also use Eq. (54) to predict the results of higher-order invariants. For example, all seventh and eighth order Z-invariants must be proportional to I_{6Z} (a result that we have confirmed by limited scanning). However, a new Z-invariant arises at ninth order, which in the $\lambda_7 = -\lambda_6$ basis must have an imaginary part that is a linear combination of $I_{6Z} P_3(\lambda_i)$ and $(\lambda_1 - \lambda_2)^3 \mathrm{Im}[(\lambda_6^2 \lambda_5^*)^2]$, where $P_3(\lambda_i)$ is a real cubic polynomial of the λ_i. Although this is a new I-invariant, it clearly vanishes when $I_{6Z} = 0$.

Finally, Eq. (54) strongly suggests that there is only one new $2Y4Z$ I-invariant and one new $Y5Z$ I-invariant, since in each case, only one new term, $\mathrm{Im}(\lambda_6^2 \lambda_5^*)$ arises that did not appear in lower-order invariants (in the $\lambda_7 = -\lambda_6$ basis).[19]

V. IMPLICATIONS FOR SPONTANEOUS *CP* VIOLATION

If a Higgs potential is explicitly CP conserving, then there exists a so-called real basis in which all the Higgs potential parameters are real. A theory with an explicitly CP-conserving Higgs sector may be CP violating if the vacuum does not respect the CP symmetry. In this case, we say that CP is spontaneously broken [5]. To determine whether CP is spontaneously broken, one must check whether the vacuum is invariant under time reversal. We assert the following theorem, which is proved in Appendix F:

Theorem 3.—Given an explicitly CP-conserving Higgs potential, the vacuum is time-reversal invariant if and only if a real basis exists in which the Higgs vacuum expectation values are real.

Theorem 3 requires one to verify the existence or nonexistence of a basis with certain properties. However, these theorems can be reformulated in a basis-independent language. Here, we follow Ref. [11], and introduce three U(2) invariants [6]:

$$-\frac{1}{2} v^2 J_1 \equiv \hat{v}^*_{\bar{a}} Y_{a\bar{b}} Z^{(1)}_{b\bar{d}} \hat{v}_d, \tag{55}$$

$$\frac{1}{4} v^4 J_2 \equiv \hat{v}^*_{\bar{b}} \hat{v}^*_{\bar{c}} Y_{b\bar{e}} Y_{c\bar{f}} Z_{e\bar{a}f\bar{d}} \hat{v}_a \hat{v}_d, \tag{56}$$

$$J_3 \equiv \hat{v}^*_{\bar{b}} \hat{v}^*_{\bar{c}} Z^{(1)}_{b\bar{e}} Z^{(1)}_{c\bar{f}} Z_{e\bar{a}f\bar{d}} \hat{v}_a \hat{v}_d, \tag{57}$$

where $\langle \Phi^0_a \rangle \equiv v \hat{v}_a / \sqrt{2}$, with $v = 246$ GeV and $\hat{v}$ is a unit vector in the complex two-dimensional Higgs flavor space. The scalar potential minimum condition is easily derived from Eq. (16):

$$\hat{v}^*_{\bar{a}} \left[Y_{a\bar{b}} + \frac{1}{2} v^2 Z_{a\bar{b}c\bar{d}} \hat{v}^*_{\bar{c}} \hat{v}_d \right] = 0. \tag{58}$$

[18]Formally, the weight $w = w(x)$ for any scalar potential parameter x is defined such that $x \to e^{iw\theta} x$ under a redefinition of one of the scalar fields by $\Phi_1 \to e^{i\theta} \Phi_1$. Of course, $w = 0$ for any real scalar potential parameter.

[19]Unfortunately, this argument fails to explain the existence of only one $3Y3Z$ I-invariant, a fact that has been confirmed only by a complete scan over all possible invariants of this type.

Thus, we may eliminate Y in the expressions for J_1 and J_2:

$$J_1 \equiv \hat{v}^*_{\bar{a}}\hat{v}^*_{\bar{e}} Z_{a\bar{b}e\bar{f}} Z^{(1)}_{b\bar{d}} \hat{v}_d \hat{v}_f, \tag{59}$$

$$J_2 \equiv \hat{v}^*_{\bar{b}}\hat{v}^*_{\bar{c}}\hat{v}^*_{\bar{g}}\hat{v}^*_{\bar{p}} Z_{b\bar{e}g\bar{h}} Z_{c\bar{f}p\bar{r}} Z_{e\bar{a}f\bar{d}} \hat{v}_a \hat{v}_d \hat{v}_h \hat{v}_r. \tag{60}$$

Since $\mathrm{Im}Y_{12}$ is determined by the scalar potential minimum conditions in terms of $\mathrm{Im}\lambda_{5,6,7}$, one is left with three potentially complex parameters in a basis where $\hat{v}$ is real. These are in one-to-one correspondence with J_1, J_2 and J_3.

Theorem 4.—Consider the 2HDM scalar potential in some arbitrary basis. Assume that the minimum of the scalar potential preserves $\mathrm{U}(1)_{\mathrm{EM}}$. Then, the Higgs sector is *CP* conserving (i.e., no explicit nor spontaneous *CP* violation is present) if J_1, J_2 and J_3 defined in Eqs. (55)–(57) are real [11].

If the Higgs sector is *CP* conserving, then according to Theorem 3 some basis must exist in which the Higgs potential parameters and the Higgs field vacuum expectation values are simultaneously real. But in that case, we may immediately conclude that the invariant quantities J_1, J_2 and J_3 must be real. Conversely, the reality of J_1, J_2 and J_3 provides sufficient conditions for a *CP*-invariant Higgs sector. This result is proven in Refs. [4,11],[20] and we do not repeat the proof here.

Note that Eqs. (55)–(57) are considerably simpler than the invariants that govern explicit *CP* violation of the Higgs potential [Eqs. (23)–(26)]. However, these two sets of invariants serve different purposes. To answer the question of whether the Higgs sector is *CP* invariant, one must first choose a basis and minimize the scalar potential. Having found $\hat{v}_a$, one may now compute J_1, J_2 and J_3. If these invariants are all real, then the Higgs potential is explicitly *CP* invariant and there is no spontaneous *CP* violation. If at least one of the invariants J_1, J_2 and J_3 is complex, then the Higgs sector is *CP* violating. However, in this latter case, one must evaluate the four I-invariants given in Eqs. (23)–(26) to determine whether *CP* is spontaneously or explicitly broken. If these four I-invariants all vanish, then *CP* is spontaneously broken. If at least one of these is nonzero, then *CP* is explicitly broken. These conclusions are summarized in our final theorem:

Theorem 5.—The necessary and sufficient conditions for spontaneous *CP* violation in the 2HDM are (i) $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = I_{3Y3Z} = 0$, and (ii) at least one of the three invariants J_1, J_2, and/or J_3 possesses a nonvanishing imaginary part. If (i) is *not* satisfied then (ii) is necessarily true, and the *CP* violation is explicit. If (ii) is *not* satisfied, then (i) is necessarily true, and the Higgs sector is *CP* conserving.

We provide two simple examples. First, Ref. [15] considers a model in which $m^2_{12} = \lambda_6 = \lambda_7 = 0$ and λ_5 is real and positive. Minimizing the scalar potential yields a purely imaginary v_2/v_1. Nevertheless, a simple relative phase redefinition of the two Higgs fields by $\pi/2$ yields a real basis with real vacuum expectation values. (In the new basis, $\lambda'_5 < 0$ and all other Higgs potential parameters are unmodified.) Hence, this model is *CP* conserving.

Second, consider a Higgs potential that satisfies Eq. (36), with λ_6 real, which was proposed in Ref. [14]. That is, all scalar potential parameters of this model are real, and the Higgs potential is explicitly *CP* conserving. In this case, a minimum of the scalar potential exists where $v_1 = v_2$ and the relative phase of the two vevs, $\xi \neq 0$. That is, we may write $\sqrt{2}\hat{v} = (e^{-i\xi/2}, e^{i\xi/2})$. Nevertheless, Ref. [14] proved that this model is *CP* conserving. We may explicitly verify this assertion by performing a U(2) transformation given by Eq. (4) with $\psi = \xi/2$, $\chi = \pi/2$ and $\theta = \pi/4$. We find that $\lambda'_5 = -\lambda_5$, $m'^2_{12} = m^2_{12}\sin\xi$, $\lambda'_6 = \lambda'_7 = \lambda_6 \sin\xi$ are all real and $\hat{v}' = (1, 0)$. Thus, we have established a basis in which all scalar potential parameters and the vacuum expectation values are simultaneously real.

Of course, the absence of spontaneous *CP* breaking in both examples can also be confirmed by checking that the invariants J_1, J_2 and J_3 are all real.

VI. CONCLUSIONS

The connection between the *CP* property of a general scalar potential and the parameters of the potential and vacuum expectation values of the Higgs fields is governed by two well-known theorems. The first, proven here as Theorem 1, states that the Higgs sector is explicitly *CP* conserving if and only if there exists a real basis, that is choice of basis (in the Higgs flavor space) in which all the scalar potential parameters are real. The second theorem, proven here as Theorem 3, states that the vacuum is *CP* invariant, implying the absence of both explicit and spontaneous *CP* violation, if and only if there exists a real basis in which the Higgs vacuum expectation values are real. In this paper, we have established a simple procedure for determining whether or not a general 2HDM is explicitly *CP* conserving by employing a set of four potentially complex basis-independent invariant combinations of the Higgs potential parameters. At least one of these invariants possesses a nonvanishing imaginary part if and only if no real basis exists.

The imaginary parts of the four complex basis-independent invariants that govern the explicit *CP*-violation properties of the 2HDM scalar potential are I_{Y3Z} [Eq. (39)], I_{2Y2Z} [Eq. (41)], I_{6Z} [Eq. (47)] and

[20] In fact, there are at most two independent relative phases among J_1, J_2 and J_3. However, as shown in Ref. [6], there are cases where two of the three invariants are real and only one has a nonvanishing imaginary part, which shows that one must check all three invariants in order to determine whether the Higgs sector is *CP* invariant.

I_{3Y3Z} [Eq. (48)]. We have shown that a real basis exists, implying that the 2HDM potential is explicitly *CP* conserving, if and only if $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = I_{3Y3Z} = 0$. We refer to these invariant imaginary parts as *I*-invariants.

Note that the above conditions are not sufficient to guarantee that the scalar sector conserves *CP*, since the minimization of the scalar potential may generate complex vevs. As stated above, if the vevs possess a nonzero relative phase in *all* real basis choices, then the model spontaneously breaks *CP*. One can formulate basis-independent conditions for spontaneous *CP* violation. First, one must prove that the Higgs sector is explicitly *CP* conserving (the corresponding invariant conditions have been given above). Spontaneous *CP* violation depends on the properties of the Higgs field vevs, v_a, which can be combined with the Higgs potential parameters to construct additional invariant quantities. Such invariant conditions have been previously obtained in Ref. [11], and are exhibited in Sec. V. Combining the information from these two classes of invariant conditions, one can distinguish between explicit and spontaneous *CP* violation in the 2HDM.

The phenomenological consequences of our invariants will be considered in a forthcoming paper. To apply the basis-independent technology to experimental studies, one would have to examine various *CP*-violating observables and express them in terms of our invariant quantities. The CERN LHC would provide the first possible arena for such studies. However, the number of Higgs observables that could be extracted from LHC analyses is limited. We anticipate that Higgs-mediated *CP*-violating effects are likely to be small, and their extraction will surely require precision measurements. A future high energy e^+e^- linear collider such as the International Linear Collider could provide the required luminosity and precision to begin a program of *CP*-violating Higgs phenomenology. We plan on examining possible *CP*-violating observables and determining their sensitivity to the *I*-invariants. This analysis will require a better understanding of the relation of the *I*-invariants to the mixing of *CP*-even/*CP*-odd neutral Higgs boson eigenstates.

Perhaps the most attractive 2HDM model is the one associated with the MSSM [16]. Indeed, the tree-level Higgs sector of the MSSM is *CP* conserving. However, when loop effects are included, supersymmetry-breaking effects, which enter via the loops, can impart nontrivial phases to parameters of the effective 2HDM scalar potential [13,17].[21] One can therefore express the *I*-invariants in terms of fundamental MSSM parameters. This may lead to relations among the four *I*-invariants introduced above, depending on the model of supersymmetry breaking.

Ultimately, if nature employs a 2HDM as an effective theory of electroweak symmetry breaking, it will be crucial to determine whether Higgs-mediated *CP* violation exists and determine its structure. By devising experimental probes of the four *I*-invariants, we hope to provide a model-independent technique for elucidating the fundamental theory that is responsible for Higgs sector dynamics.

[21]These phases would be directly related to phases of fundamental complex MSSM parameters such as the supersymmetric-conserving μ term and the supersymmetry-breaking gaugino Majorana mass terms and matrix *A* parameters.

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APPENDIX A: EXISTENCE OF A REAL BASIS

In this Appendix, we prove Theorem 1 that was quoted at the beginning of Sec. III.

Theorem 1.—The Higgs potential is explicitly *CP* conserving if and only if a basis exists in which all Higgs potential parameters are real. Otherwise, *CP* is explicitly violated.

A basis in which all Higgs potential parameters are real will be called a real basis. In order to prove Theorem 1, one can either consider the most general *CP* transformation laws of the scalar fields or invoke the *CPT* theorem [18] and consider the most general scalar field transformation laws under time reversal. Here we choose the latter procedure.[22] Following Ref. [19], we note that the form for the action of the antiunitary time-reversal operator $\mathcal{T}$ on a set of scalar field multiplets is given by

$$\begin{aligned} \mathcal{T}\,\Phi_a(\vec{x},t)\mathcal{T}^{-1} &= e^{i\psi}(U_T)_{a\bar{b}}\Phi_b(\vec{x},-t), \\ \mathcal{T}\Phi^\dagger_{\bar{a}}(\vec{x},t)\mathcal{T}^{-1} &= \Phi^\dagger_{\bar{b}}(\vec{x},-t)(U^\dagger_T)_{b\bar{a}}e^{-i\psi}, \end{aligned} \tag{A1}$$

where U_T is a *symmetric* unitary matrix that depends on the choice of basis. The arbitrary phase factor $e^{i\psi}$ corresponds to the freedom to make $\mathrm{U}(1)_Y$ transformations.[23] To prove that U_T is symmetric, we apply the time-reversal operator twice and use the well-known result that $\mathcal{T}^2\Phi_a(\vec{x},t)\mathcal{T}^{-2} = \Phi_a(\vec{x},t)$; that is, $\mathcal{T}^2 = 1$ when applied to a bosonic field [20]. Applying this result to Eq. (A1) yields $U_T^* U_T = I$, due to the antiunitarity of $\mathcal{T}$. Since U_T

[22]In Ref. [4], the *CP* transformation of the scalar fields in the real basis is used to prove that the scalar Lagrangian is *CP* invariant.

[23]More generally, the time-reversal operator is defined modulo $\mathrm{SU}(2)\times\mathrm{U}(1)_Y$ gauge transformations that leave the Lagrangian invariant (and hence do not modify the scalar potential parameters).

is unitary, it follows that U_T must satisfy $U_T^T = U_T$. The (canonical) kinetic energy terms of the scalar field theory are automatically time-reversal invariant. It then follows that the scalar Lagrangian is time-reversal invariant if the scalar potential satisfies[24]:

$$\mathcal{T}\,\mathcal{V}(\Phi,\{p\})\mathcal{T}^{-1} = \mathcal{V}(U_T\Phi,\{p^*\}) = \mathcal{V}(\Phi,\{p\}), \quad \text{(A2)}$$

where $\{p\}$ represents the Higgs potential parameters appearing in $\mathcal{V}$, and the complex conjugated parameters $\{p^*\}$ appear above due to the antiunitarity of $\mathcal{T}$. If Eq. (A2) is satisfied, then the action is invariant under time-reversal transformations.

Suppose that a basis exists in which all the Higgs potential parameters are real. In this case, we may choose $U_T = 1$, in which case Eq. (A2) is trivially satisfied. To complete the proof of Theorem 1, we must show that a basis exists in which all the Higgs potential parameters are real if Eq. (A2) is satisfied. First, we examine the quadratic part of the Higgs potential, which we can write in matrix notation as

$$\mathcal{V}_2 = \Phi^\dagger Y \Phi, \quad \text{(A3)}$$

where Y is a Hermitian matrix. Time-reversal invariance of $\mathcal{V}_2$ requires

$$\mathcal{T}\,\Phi^\dagger Y \Phi \mathcal{T}^{-1} = \Phi^\dagger U_T^\dagger Y^* U_T \Phi = \Phi^\dagger Y \Phi, \quad \text{(A4)}$$

where we have used $\mathcal{T} Y \mathcal{T}^{-1} = Y^*$. Equation (A4) implies that

$$U_T^\dagger Y^* U_T = Y. \quad \text{(A5)}$$

As shown in Appendix B, since U_T is unitary and symmetric, we can write

$$U_T = V^T V, \quad \text{(A6)}$$

where V is unitary (but not necessarily symmetric). As a result, Eq. (A5) will be true if

$$V^\dagger V^* Y^* V^T V = Y, \quad \text{(A7)}$$

which can be converted to

$$(V Y V^\dagger)^* = V Y V^\dagger. \quad \text{(A8)}$$

That is $Y' \equiv V Y V^\dagger$ is real. But, Y' is simply Y in the new basis $\Phi' = V\Phi$. Thus, there exists a basis in which the parameters of $\mathcal{V}_2$ are real.

A similar computation can be performed for the rest of the terms appearing in the scalar potential. In particular, if we write the quartic part of the Higgs potential as

$$\mathcal{V}_4 = \frac{1}{2} Z_{a\bar{b}c\bar{d}} (\Phi_{\bar{a}}^\dagger \Phi_b)(\Phi_{\bar{c}}^\dagger \Phi_d), \quad \text{(A9)}$$

then the analog of Eq. (A5) is

$$(U_T^\dagger)_{e\bar{a}} (U_T)_{b\bar{f}} (U_T^\dagger)_{g\bar{c}} (U_T)_{d\bar{h}} Z^*_{a\bar{b}c\bar{d}} = Z_{e\bar{f}g\bar{h}}. \quad \text{(A10)}$$

We again apply Eq. (A6) and conclude that

$$[V_{p\bar{a}} V^\dagger_{b\bar{q}} V_{r\bar{c}} V^\dagger_{d\bar{s}} Z_{a\bar{b}c\bar{d}}]^* = V_{p\bar{e}} V^\dagger_{f\bar{q}} V_{r\bar{g}} V^\dagger_{h\bar{s}} Z_{e\bar{f}g\bar{h}}. \quad \text{(A11)}$$

That is, the unitary transformation V produces the basis in which *all* the Higgs potential parameters are real.

Conversely, if no basis exists in which the Higgs potential parameters are real, then no unitary matrix V exists such that Eqs. (A8) and (A11) are simultaneously satisfied. Following the above proof in the backward direction, one can conclude that no choice of a unitary symmetric matrix U_T exists that satisfies Eq. (A2).

In some cases (see below), more than one suitable time-reversal operator exists. Any one of these operators can be used to demonstrate that the Higgs potential is explicitly CP invariant. Nevertheless, in order to ascertain that the Higgs sector is invariant under CP, it is necessary to verify that the vacuum is also CP invariant (equivalently time-reversal invariant). In particular, the vacuum may select out a unique time-reversal operator, as shown in Appendix F. (If the vacuum is noninvariant with respect to all possible candidate time-reversal operators, then time-reversal invariance is spontaneously broken.) Thus, it is important to consider the possible nonuniqueness in the definition of $\mathcal{T}$ given in Eq. (A1).

For an explicitly CP-conserving Higgs potential, a real basis must exist. However, the real basis is not unique. In particular, given a real Φ'-basis, there exists an $\mathrm{O}(2) \times \mathcal{D}$ subgroup of U(2) consisting of 2×2 unitary matrices $W_{a\bar{b}}$ such that the scalar potential parameters remain real under $\Phi'_a \to \Phi''_a = W_{a\bar{b}} \Phi'_b$. Here, $\mathcal{D}$ is the maximal discrete subgroup of U(2) that is a symmetry of the Higgs Lagrangian. In addition, one is free to make $\mathrm{U}(1)_Y$ phase rotations, which simply reflects the fact that U_T is only defined up to an overall phase. If $\mathcal{D}$ is trivial, then W is an orthogonal transformation and $U_T = I$ (up to an overall phase) in *any* real basis. If $\mathcal{D}$ is nontrivial, then $W^T W \neq e^{i\eta} I$ (for any phase choice η), in which case the choice of U_T in the definition of the time-reversal operator is not unique (modulo gauge transformations).

To amplify these remarks, we suppose that in the original Φ-basis another antiunitary operator $\tilde{\mathcal{T}}$ exists that is a potential candidate for the time-reversal operator. In particular, suppose that there exists a symmetric unitary matrix $\tilde{U}_T \neq e^{i\eta} U_T$ such that[25]

$$\begin{aligned} \tilde{\mathcal{T}} \Phi_a(\vec{x}, t) \tilde{\mathcal{T}}^{-1} &= e^{i\tilde{\psi}} (\tilde{U}_T)_{a\bar{b}} \Phi_b(\vec{x}, -t), \\ \mathcal{V}(\Phi, \{p\}) &= \mathcal{V}(\tilde{U}_T \Phi, \{p^*\}). \end{aligned} \quad \text{(A12)}$$

Then, the analysis above implies that there exists a unitary

[24]We henceforth omit exhibiting the explicit dependence of the fields on the space-time coordinates.

[25]That is, if $\tilde{U}_T \neq U_T$ in the Φ-basis, for any choices of the phases $\tilde{\psi}$ and ψ, then $\tilde{\mathcal{T}}$ and $\mathcal{T}$ are distinct and equally valid choices for the time-reversal operator.

matrix $\tilde{V}$ such that $\tilde{U} = \tilde{V}^T\tilde{V}$, and $\Phi'' = \tilde{V}\Phi$ is also a real basis. In this case, the real Φ'-basis and the real Φ''-basis are related by $\Phi'' = W\Phi'$ where $W = \tilde{V}V^{-1}$. It follows that $WW^T = \tilde{V}U^{-1}\tilde{V}^T \neq e^{i\eta}I$ (for any phase choice η). Thus, the existence of $\tilde{\mathcal{T}} \neq \mathcal{T}$ implies that the discrete group $\mathcal{D}$ is nontrivial. Likewise, one can show that $W^TW = [V^{-1}]^T\tilde{U}V^{-1} \neq e^{i\eta}I$.

Given U_T in the Φ-basis, we may determine the form of U_T in any real basis. For example, inserting $\Phi' = V\Phi$ into Eq. (A1) and making use of Eq. (A6), we find

$$\mathcal{T}\,\Phi'_a(\vec{x}, t)\mathcal{T}^{-1} = e^{i\psi}\Phi'_a(\vec{x}, -t). \tag{A13}$$

That is, in the Φ'-basis, $U'_T = I$. Equation (A2) then implies that this is a real basis. Now, let us transform to the real basis $\Phi'' = W\Phi'$. A similar computation yields

$$\mathcal{T}\,\Phi''_a(\vec{x}, t)\mathcal{T}^{-1} = e^{i\psi}(WW^T)^{-1}_{a\bar{b}}\Phi''_b(\vec{x}, -t), \tag{A14}$$

where $U''_T = (WW^T)^{-1} \neq I$ in the Φ''-basis. Similarly, if we identify $\tilde{\mathcal{T}}$ as the time-reversal operator, we find that $\tilde{U}'_T = W^TW \neq I$ and $\tilde{U}''_T = I$. We may assemble all possible real bases into classes. Each class is in one-to-one correspondence with the elements of the discrete group $\mathcal{D}$. In the class of real bases associated with the identity element of $\mathcal{D}$, the corresponding $U_T = I$. In all other classes of real bases, the corresponding $U_T \neq I$.

If $\mathcal{D}$ is trivial, so that W is an orthogonal transformation [up to an overall phase that can be absorbed, e.g., into the multiplicative phase factor in Eq. (A14)], then $U_T = I$ in *any* real basis. In this case, the definition of the time-reversal operator $\mathcal{T}$ is unique (modulo gauge transformations).

Finally, we note that the existence of a nontrivial discrete subgroup $\mathcal{D}$ imposes strong constraints on the parameters of the Higgs potential. Consider a real Φ'-basis and a real Φ''-basis related by $\Phi'' = W\Phi'$. It then follows that $Y'' = WY'W^\dagger$. By assumption, Y' and Y'' are real. A short computation then yields the vanishing of the following commutators:

$$[Y', W^TW] = [Y'', WW^T] = 0. \tag{A15}$$

A similar constraint arises from the requirement that both Z' and Z'' are real. Using these results, it is straightforward to verify that Eq. (A12) is satisfied for $\tilde{U}'_T = W^TW$ in the Φ'-basis and Eq. (A2) is satisfied for $U''_T = (WW^T)^{-1}$ in the Φ''-basis.

APPENDIX B: A PROOF OF A RESULT FROM MATRIX ANALYSIS

In the proof of Theorems 1 and 4, the following lemma is required:

Lemma 1.—A complex $n \times n$ matrix U is unitary and symmetric if and only if there is a complex $n \times n$ unitary matrix V such that $U = V^TV$.

This result is given as problem 17 on p. 215 of Ref. [21]. Here, we give an explicit proof. Clearly if V is unitary it follows that U is unitary and symmetric. Thus, we focus on the proof that given U, the unitary matrix V exists. Lemma 1 is a special case of the Takagi factorization of a complex symmetric matrix (see pp. 204–206 of Ref. [21]). Namely, for any complex symmetric matrix M, there exists a unitary matrix V such that $M = V^TDV$, where D is a real non-negative diagonal matrix whose elements are given by the non-negative square roots of the eigenvalues of $MM^\dagger$.[26] Applying the Takagi factorization to a unitary matrix $M = U$ (i.e., $UU^\dagger = I$), it immediately follows that $D = I$. Hence, $U = V^TV$ for some unitary matrix V.

The matrix V is not unique. In particular, if $U = V^TV$ then $U = W^TW$, where the unitary matrix $W = KV$ and K is an arbitrary orthogonal matrix. However, the proof of Theorem 4 simply requires the existence of V, which has been proven above.

APPENDIX C: DOES A BASIS EXIST IN WHICH ALL THE λ_i ARE REAL?

Lemma 2.—If the parameters of the 2HDM satisfy the relations, $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$, then one can always transform to a new basis in which λ'_5 and $\lambda'_7 = -\lambda'_6$ are all real.

We begin with Eqs. (12) and (13) and require that the imaginary parts of λ'_5 and λ'_6 are zero. We assume that $\lambda_6 \neq 0$ (if $\lambda_7 = -\lambda_6 = 0$, it is trivial to transform to a basis where λ_5 is real by rephasing one of the scalar fields). Moreover, without loss of generality, we may assume that λ_6 is real by rephasing one of the scalar fields appropriately.[27] If λ_5 is also real after the rephasing, we are done. If not, we write $\lambda_5 \equiv |\lambda_5|e^{i\theta_5}$ and obtain

$$\mathrm{Im}\,\lambda'_5 = -\frac{1}{2}f_b\sin 2\chi + f_a\cos 2\chi, \tag{C1}$$

$$\mathrm{Im}\,\lambda'_6 = -\frac{1}{4}f_d\sin\chi + \frac{1}{2}f_c\cos\chi, \tag{C2}$$

where

$$f_a = |\lambda_5|c_{2\theta}\sin(\theta_5 + 2\xi) - 2\lambda_6 s_{2\theta}\sin\xi, \tag{C3}$$

$$f_b = (\lambda_1 - \lambda_3 - \lambda_4)s^2_{2\theta} + |\lambda_5|(2 - s^2_{2\theta})\cos(\theta_5 + 2\xi) - 2\lambda_6 s_{4\theta}\cos\xi, \tag{C4}$$

$$f_c = |\lambda_5|s_{2\theta}\sin(\theta_5 + 2\xi) + 2\lambda_6 c_{2\theta}\sin\xi, \tag{C5}$$

[26] The Takagi factorization of a complex symmetric matrix is the basis for the mass diagonalization of a general Majorana fermion mass matrix [22].

[27] Since $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$, it follows that $\lambda'_7 = -\lambda'_6$, and further consideration of λ_7 is unnecessary.

$$f_d = [|\lambda_5|\cos(\theta_5 + 2\xi) - \lambda_1 + \lambda_3 + \lambda_4)]s_{4\theta} + 4\lambda_6 c_{4\theta}\cos\xi. \tag{C6}$$

As before, we abbreviate $s_{4\theta} \equiv \sin 4\theta$, $c_{4\theta} \equiv \cos 4\theta$, etc. We proceed to solve $\mathrm{Im}\lambda_5' = 0$, which yields an equation for $\cot 2\chi$, and $\mathrm{Im}\lambda_6' = 0$, which yields an equation for $\cot\chi$:

$$\cot 2\chi = \frac{f_b}{2f_a}, \tag{C7}$$

$$\cot\chi = \frac{f_d}{2f_c}. \tag{C8}$$

Under the assumption that $f_a \neq 0$ and $f_c \neq 0$, we can eliminate χ by employing the well-known identity

$$\cot 2\chi = \frac{\cot^2\chi - 1}{2\cot\chi}, \tag{C9}$$

which leads to the following result:

$$G(\theta, \xi) \equiv f_a(f_d^2 - 4f_c^2) - 2f_b f_c f_d = 0. \tag{C10}$$

We wish to prove that there exists at least one θ and ξ that solves Eq. (C10). From any such solution, we may compute χ from Eqs. (C7) and (C8). This would then provide the elements of the U(2) transformation matrix that yields the basis in which all the λ_i are real.

To prove that a solution to $G(\theta, \xi) = 0$ exists, we note that

$$f_a(\theta = 0, \xi) = -f_a(\theta = \pi/2, \xi) = |\lambda_5|\sin(\theta_5 + 2\xi), \tag{C11}$$

$$f_b(\theta = 0, \xi) = +f_b(\theta = \pi/2, \xi) = 2|\lambda_5|\cos(\theta_5 + 2\xi), \tag{C12}$$

$$f_c(\theta = 0, \xi) = -f_c(\theta = \pi/2, \xi) = 2\lambda_6\sin\xi, \tag{C13}$$

$$f_d(\theta = 0, \xi) = +f_d(\theta = \pi/2, \xi) = 4\lambda_6\cos\xi, \tag{C14}$$

from which it follows that

$$G(0, \xi) = -G(\pi/2, \xi) = 16\lambda_6^2|\lambda_5|\sin\theta_5. \tag{C15}$$

This means that G will have at least one sign change as a function of θ. Hence, for any value of ξ there exists a value of θ for which $G(\theta, \xi) = 0$. Thus, we have proved the existence of a U(2) transformation that results in a basis in which all the λ_i are real.

The assumption above that $f_a \neq 0$ and $f_c \neq 0$ for values of θ and ξ at which $G(\theta, \xi) = 0$ is not strictly necessary. For example, if $f_a = 0$ (but $f_b \neq 0$), then one can rewrite Eq. (C7) in terms of $\tan 2\chi$. We then end up again with Eq. (C10). The only special cases that need be considered are (i) $f_a = f_b = 0$ and (ii) $f_c = f_d = 0$. If (i) and (ii) both hold, then we immediately conclude that λ_5' and λ_6' are real and we are finished. If only (i) [only (ii)] holds, then we simply use Eq. (C8) [Eq. (C7)] to determine χ, and we are finished.

We have used Lemma 2 in the proof of Theorem 2 (see Sec. III). It is instructive to examine the necessity of the condition of $\lambda_1 = \lambda_2$ in the proof of Lemma 2. For this reason, we prove a second lemma.

Lemma 3.—If $\lambda_1 \neq \lambda_2$ and $\mathrm{Im}(\lambda_5^*\lambda_6^2) \neq 0$ in a basis where $\lambda_7 = -\lambda_6 \neq 0$, then it is impossible to transform to a basis in which λ_5', λ_6' and λ_7' are all real.

The proof of Lemma 3 is trivial using invariants. Namely, in a basis where $\lambda_7 = -\lambda_6 \neq 0$, we use Eq. (30) to conclude that $I_{6Z} \neq 0$. Hence in this case, there is no basis in which all the λ_i are real.

Even without invariants, it is not difficult to show that no basis exists in which all the λ_i are real. We first rephase one of the scalar fields such that the resulting value of λ_6 is real. In this basis, $\lambda_5 \equiv |\lambda_5|e^{i\theta_5}$, where $\theta_5 \neq 0(\mathrm{mod}\,\pi)$. We then use Eqs. (13) and (14) in the case of $\lambda_7 = -\lambda_6$ to obtain

$$\mathrm{Im}\,(\lambda_6' + \lambda_7') = \frac{1}{2}\sin\chi s_{2\theta}(\lambda_1 - \lambda_2). \tag{C16}$$

Since $\lambda_1 \neq \lambda_2$, it follows that $\mathrm{Im}\lambda_6' = \mathrm{Im}\lambda_7' = 0$ implies that either $\sin 2\theta = 0$ or $\sin\chi = 0$.

If $\sin 2\theta = 0$, then Eqs. (12) and (13) yield

$$\lambda_5' e^{2i\chi} = |\lambda_5|e^{\pm i(2\xi + \theta)}, \tag{C17}$$

$$\lambda_6' e^{i\chi} = |\lambda_5|e^{\pm i\theta}, \tag{C18}$$

where the choice of sign above corresponds to the sign of $\cos 2\theta$. Thus,

$$\frac{\lambda_5'}{\lambda_6'^2} = \frac{|\lambda_5|}{\lambda_6^2}e^{\pm i\theta_5}, \tag{C19}$$

and we see that no basis exists in which λ_5' and λ_6' are simultaneously real.

Next, suppose that $\sin 2\theta \neq 0$ and $\sin\chi = 0$. Equations (12) and (13) then yield

$$\mathrm{Im}\,(\lambda_5') = |\lambda_5|c_{2\theta}\sin(\theta_5 + 2\xi) - 2\lambda_6 s_{2\theta}\sin\xi, \tag{C20}$$

$$\mathrm{Im}\,(\lambda_6') = \frac{1}{2}|\lambda_5|s_{2\theta}\sin(\theta_5 + 2\xi) + \lambda_6 c_{2\theta}\sin\xi. \tag{C21}$$

If $\sin\xi = 0$, then $\mathrm{Im}(\lambda_6') = \frac{1}{2}|\lambda_5|\sin 2\theta\sin\theta_5 \neq 0$. Thus, $\sin\xi \neq 0$ if λ_6' is real. Using Eqs. (C20) and (C21) to set $\mathrm{Im}(\lambda_5') = \mathrm{Im}(\lambda_6') = 0$ yields

$$\tan 2\theta = -\cot 2\theta = \frac{|\lambda_5|\sin(\theta_5 + 2\xi)}{2\lambda_6\sin\xi}. \tag{C22}$$

However, Eq. (C22) implies that $\tan^2 2\theta = -1$, which is impossible. Once again, we conclude that no basis exists in which λ_5' and λ_6' are simultaneously real. The proof of Lemma 3 is now complete.

APPENDIX D: PROOF OF LEMMA 4

Consider the special isolated point of the Higgs parameter space in which $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$. By Lemma 2, we may assume without loss of generality that all the λ_i are real. Thus, Y_{12} remains as the only potentially complex parameter. Lemma 4 provides the conditions under which it is possible to find a new basis in which all the Higgs potential parameters are real.

Lemma 4.—If the parameters of the 2HDM satisfy the relations, $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$, and the basis is chosen such that all the λ_i are real and Y_{12} is complex, then there exists a new basis in which all the Higgs potential parameters are real if and only if (at least) one of the following two conditions is satisfied:

$$\lambda_5^2 + \lambda_5(\lambda_1 - \lambda_3 - \lambda_4) - 2\lambda_6^2 = 0, \tag{D1}$$

and/or

$$4\lambda_6(\mathrm{Re}Y_{12})^2 - (\lambda_3 + \lambda_4 + \lambda_5 - \lambda_1)(Y_{11} - Y_{22})\mathrm{Re}Y_{12} - \lambda_6(Y_{11} - Y_{22})^2 = 0. \tag{D2}$$

It is easy to prove that if neither Eq. (D1) nor Eq. (D2) is satisfied, then there is no basis in which all Higgs potential parameters are real. The latter conclusion follows directly from $I_{3Y3Z} \neq 0$, which is a consequence of Eq. (32). Thus, we focus on the inverse statement: if either Eq. (D1) or Eq. (D2) is satisfied, then there exists a basis in which all the Higgs potential parameters are real.

Suppose that Eq. (D1) is satisfied, under the assumption that all the λ_i are real (for $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$) and Y_{12} is complex. We search for a U(2) transformation to a new basis in which the λ_i' and Y_{12}' are real. It will be sufficient to consider solutions with $\chi = \pi/2$. At this point, we assume that $\lambda_6 \neq 0$ (we shall treat the case of $\lambda_6 = 0$ separately). Then, we demand that θ is the solution (as a function of ξ) of the following equation:

$$\lambda_6 \sin 2\theta = \lambda_5 \cos 2\theta \cos\xi. \tag{D3}$$

Using Eq. (C1) with $\chi = \pi/2$ and real λ_5, it is easy to check that Eq. (D3) implies that $\mathrm{Im}\lambda_5' = 0$. Next, using Eq. (C2) with $\chi = \pi/2$ and real λ_5 yields

$$\mathrm{Im}\,\lambda_6' = -\frac{1}{4}(\lambda_5 \cos 2\xi - \lambda_1 + \lambda_3 + \lambda_4)\sin 4\theta - \lambda_6 \cos 4\theta \cos\xi. \tag{D4}$$

Using Eq. (D3), we obtain

$$\sin 4\theta = 2\sin 2\theta \cos 2\theta = \frac{2\lambda_5 \cos^2 2\theta \cos\xi}{\lambda_6}, \tag{D5}$$

$$\cos 4\theta = \cos^2 2\theta - \sin^2 2\theta = \cos^2 2\theta\left(1 - \frac{\lambda_5^2 \cos^2\xi}{\lambda_6^2}\right). \tag{D6}$$

Inserting these results into Eq. (D4) and simplifying the resulting expression yields

$$\mathrm{Im}\,\lambda_6' = \frac{\cos^2 2\theta \cos\xi}{2\lambda_6}[\lambda_5^2 + \lambda_5(\lambda_1 - \lambda_3 - \lambda_4) - 2\lambda_6^2]. \tag{D7}$$

Thus, using Eq. (D1), we see that $\mathrm{Im}\lambda_6' = 0$ for *any* value of ξ. We now choose ξ in order that $\mathrm{Im}Y_{12}' = 0$. Using Eq. (7) with $\chi = \pi/2$ and $Y_{12} \equiv |Y_{12}|e^{i\theta_{12}}$, we find

$$2|Y_{12}|\cos 2\theta \cos(\theta_{12} + \xi) = (Y_{11} - Y_{22})\sin 2\theta. \tag{D8}$$

Using Eq. (D3) to eliminate θ, we end up with

$$\tan\xi = \cot\theta_{12} - \frac{\lambda_5(Y_{11} - Y_{22})}{2\lambda_6|Y_{12}|\sin\theta_{12}}. \tag{D9}$$

Finally, we treat the case of $\lambda_6 = 0$. We may assume that $\lambda_5 \neq 0$ (otherwise, a simple rephasing of one of the Higgs fields is sufficient to yield a real Y_{12}). In this case, we choose $\chi = \xi = \pi/2$. Then, $\mathrm{Im}\lambda_5' = 0$ is satisfied [see Eq. (D3)] for arbitrary θ. Inserting $\xi = \pi/2$ into Eq. (D4) yields

$$\mathrm{Im}\,\lambda_6' = \frac{1}{4}(\lambda_5 + \lambda_1 - \lambda_3 - \lambda_4)\sin 4\theta = 0, \tag{D10}$$

after using Eq. (D1) with $\lambda_6 = 0$ and $\lambda_5 \neq 0$. We now choose θ in order that $\mathrm{Im}Y_{12}' = 0$. After putting $\xi = \pi/2$ in Eq. (D8), the end result is

$$\cot 2\theta = \frac{Y_{22} - Y_{11}}{2|Y_{12}|\sin\theta_{12}}. \tag{D11}$$

To summarize, if Eq. (D1) is satisfied, we have exhibited a U(2) transformation [Eq. (4) with $\chi = \pi/2$, θ given by the solution to Eq. (D3) and ξ given by Eq. (D9) if $\lambda_6 \neq 0$, and $\chi = \xi = \pi/2$ and θ given by the solution to Eq. (D11) if $\lambda_6 = 0$] such that all Higgs potential parameters are real in the transformed basis.[28]

Next, suppose that Eq. (D2) is satisfied, under the assumption that Y_{12} is complex and all the λ_i are real (where $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$). We again search for a U(2) transformation to a new basis in which the λ_i are still real and Y_{12} is real. In this case, we choose $\chi = \pi/2$ and $\xi = \pi$. For this choice, $\mathrm{Im}\lambda_5' = 0$ is automatic (independently of the value of θ). Again, we first assume that $\lambda_6 \neq 0$ (the case of $\lambda_6 = 0$ is treated separately). Then, the constraints $\mathrm{Im}Y_{12}' = 0$ [Eq. (D8)] and $\mathrm{Im}\lambda_6' = 0$ [Eq. (D4)] reduce to

[28]Other U(2) transformations with $\chi \neq \pi/2$ can also produce a basis where all Higgs potential parameters are real. For example, a numerical analysis suggests that if $\chi \neq 0 \pmod{\pi}$ and $\lambda_6 \neq 0$, then one can choose θ as a function of ξ such that $\mathrm{Im}\lambda_5' = 0$. Using this choice for θ, one again finds that $\mathrm{Im}\lambda_6' = 0$ as a consequence of Eq. (D1), independently of the value of ξ. Finally, ξ can be chosen to yield $\mathrm{Im}Y_{12}' = 0$. Of course, only one solution for (χ, θ, ξ) must be exhibited to prove the validity of Lemma 4.

$$\cot 2\theta = \frac{Y_{22} - Y_{11}}{2|Y_{12}|\cos\theta_{12}}, \tag{D12}$$

$$\cot 4\theta = \frac{\lambda_5 - \lambda_1 + \lambda_3 + \lambda_4}{4\lambda_6}, \tag{D13}$$

respectively. Using the double-angle formula analogous to Eq. (C9), we may combine Eqs. (D12) and (D13) to yield the following constraint:

$$4\lambda_6|Y_{12}|^2\cos^2\theta_{12} - \lambda_6(Y_{22} - Y_{11})^2 + (\lambda_5 - \lambda_1 + \lambda_3 + \lambda_4)(Y_{22} - Y_{11})|Y_{12}|\cos\theta_{12} = 0, \tag{D14}$$

which is identical to Eq. (D2), which is assumed to be satisfied. Thus, Eqs. (D12) and (D13) are consistent and provide a solution for θ.

Finally, we examine the case of $\lambda_6 = 0$. In this case, Eq. (D2) reduces to

$$(\lambda_1 - \lambda_3 - \lambda_4 - \lambda_5)(Y_{11} - Y_{22})\cos\theta_{12} = 0. \tag{D15}$$

The case of $\lambda_1 - \lambda_3 - \lambda_4 - \lambda_5 = 0$ (with $\lambda_6 = 0$) is equivalent to Eq. (D1) and has already been treated. Thus, it is sufficient to examine the cases of $Y_{11} = Y_{22}$ and $\cos\theta_{12} = 0$. In both cases, we may choose $\chi = \pi/2$ and $\xi = \pi$ as before. Then, it is easy to check that if $\cos 2\theta = 0$ in the case of $Y_{11} = Y_{22}$ and $\sin 2\theta = 0$ in the case of $\cos\theta_{12} = 0$, the U(2) transformation [Eq. (4)] yields $\mathrm{Im}\lambda'_5 = \mathrm{Im}Y'_{12} = 0$.

To summarize, if Eq. (D2) is satisfied, we have exhibited a U(2) transformation [e.g., Eq. (4) with $\chi = \pi/2$, $\xi = \pi$ and θ given by the solution to Eq. (D12) if $\lambda_6 \neq 0$] such that all Higgs potential parameters are real in the transformed basis.

Thus, we have explicitly constructed a U(2) transformation that renders all Higgs potential parameters real if either Eq. (D1) or Eq. (D2) is satisfied. Consequently, $I_{3Y3Z} = 0$, and it follows that if $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$, then the condition $I_{3Y3Z} = 0$ is the necessary and sufficient condition for an explicitly CP-conserving Higgs potential. This concludes the proof of Lemma 4.

APPENDIX E: ALL CUBIC INVARIANTS ARE REAL

In this Appendix, we examine invariants constructed from the $Y_{a\bar{b}}$ and $Z_{a\bar{b}c\bar{d}}$. We show that all invariants that are at most cubic in the Z's and independent of Y are real. Similarly, we demonstrate that invariants that are linear in Y and at most quadratic in the Z's are real. Finally, we prove that invariants that are linear in Z and quadratic in the Y's are real.

First, we introduce some notation. We consider all possible nontrivial[29] second-rank tensors that are quadratic in the Z's. Using the symmetry properties of the Z's, we find six tensors of this kind:

$$Z^{(11)}_{c\bar{d}} \equiv Z^{(1)}_{a\bar{b}} Z_{b\bar{a}c\bar{d}}, \qquad Z^{(12)}_{c\bar{d}} \equiv Z^{(1)}_{a\bar{b}} Z_{b\bar{d}c\bar{a}}, \tag{E1}$$

$$Z^{(21)}_{c\bar{d}} \equiv Z^{(2)}_{a\bar{b}} Z_{b\bar{a}c\bar{d}}, \qquad Z^{(22)}_{c\bar{d}} \equiv Z^{(2)}_{a\bar{b}} Z_{b\bar{d}c\bar{a}}, \tag{E2}$$

$$Z^{(31)}_{c\bar{d}} \equiv Z_{a\bar{b}e\bar{d}} Z_{b\bar{a}c\bar{e}}, \qquad Z^{(32)}_{c\bar{d}} \equiv Z_{a\bar{b}e\bar{d}} Z_{c\bar{a}b\bar{e}}, \tag{E3}$$

where $Z^{(1)}$ and $Z^{(2)}$ are defined in Eq. (19). A quick computation shows that the $Z^{(m)}$ ($m = 1, 2$) and the $Z^{(pn)}$ ($p = 1, 2, 3$ and $n = 1, 2$) are Hermitian; that is,

$$Z^{(m)}_{a\bar{b}} = [Z^{(m)}_{b\bar{a}}]^*, \qquad Z^{(pn)}_{a\bar{b}} = [Z^{(pn)}_{b\bar{a}}]^*. \tag{E4}$$

Next, we consider all possible nontrivial[30] fourth-rank tensors that are quadratic in the Z's. These fall into a number of different classes. First, we have

$$Z^{(1)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{b}e\bar{f}} Z_{c\bar{d}f\bar{e}}, \qquad Z^{(4)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{d}f\bar{e}} Z_{c\bar{b}e\bar{f}}, \tag{E5}$$

$$Z^{(2)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{f}e\bar{d}} Z_{f\bar{b}c\bar{e}}, \qquad Z^{(5)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{e}f\bar{b}} Z_{c\bar{f}e\bar{d}}, \tag{E6}$$

$$Z^{(3)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{f}c\bar{e}} Z_{f\bar{b}e\bar{d}}, \qquad Z^{(6)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{f}c\bar{e}} Z_{e\bar{b}f\bar{d}}. \tag{E7}$$

These fourth-rank tensors possess the same symmetry and Hermiticity properties as $Z_{a\bar{b}c\bar{d}}$, that is,

$$Z^{(n)}_{a\bar{b}c\bar{d}} = Z^{(n)}_{c\bar{d}a\bar{b}}, \qquad [Z^{(n)}_{a\bar{b}c\bar{d}}]^* = Z^{(n)}_{b\bar{a}d\bar{c}}. \tag{E8}$$

Note that $Z^{(n+3)}_{a\bar{b}c\bar{d}} \equiv Z^{(n)}_{c\bar{b}a\bar{d}}$ for $n = 1, 2, 3$. The second class of rank-four tensors consists of

$$\tilde{Z}^{(1)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{b}e\bar{f}} Z_{c\bar{e}f\bar{d}}, \qquad \tilde{Z}^{(3)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{e}f\bar{d}} Z_{c\bar{b}e\bar{f}}, \tag{E9}$$

$$\tilde{Z}^{(2)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{e}f\bar{b}} Z_{c\bar{d}e\bar{f}}, \qquad \tilde{Z}^{(4)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{d}e\bar{f}} Z_{c\bar{e}f\bar{b}}. \tag{E10}$$

Note that $\tilde{Z}^{(n+2)}_{a\bar{b}c\bar{d}} \equiv \tilde{Z}^{(n)}_{c\bar{b}a\bar{d}}$ for $n = 1, 2$. Unlike $Z_{a\bar{b}c\bar{d}}$ and $Z^{(n)}_{a\bar{b}c\bar{d}}$, the tensors $\tilde{Z}^{(n)}_{a\bar{b}c\bar{d}}$ are not symmetric under interchange of the first and second pair of indices. In particular,

$$\tilde{Z}^{(1)}_{a\bar{b}c\bar{d}} = \tilde{Z}^{(2)}_{c\bar{d}a\bar{b}}, \qquad \tilde{Z}^{(3)}_{a\bar{b}c\bar{d}} = \tilde{Z}^{(4)}_{c\bar{d}a\bar{b}}. \tag{E11}$$

Consequently, we must distinguish between two types of Hermiticity conditions. For $n = 1, 2$, the $\tilde{Z}^{(n)}_{a\bar{b}c\bar{d}}$ satisfy the Hermiticity condition of the first kind:

$$[\tilde{Z}^{(n)}_{a\bar{b}c\bar{d}}]^* = \tilde{Z}^{(n)}_{b\bar{a}d\bar{c}}, \qquad n = 1, 2, \tag{E12}$$

whereas for $n = 3, 4$, the $\tilde{Z}^{(n)}_{a\bar{b}c\bar{d}}$ satisfy the Hermiticity

[29] That is, we omit tensors that can be expressed as a product of a scalar quantity times $Z^{(m)}_{a\bar{b}}$, $m = 1, 2$ (e.g., $Z_{c\bar{c}d\bar{d}} Z_{e\bar{e}a\bar{b}} \equiv [\mathrm{Tr}Z^{(2)}]Z^{(2)}_{a\bar{b}}$).

[30] Again, we omit those tensors that are products of simpler tensors (e.g., $Z_{a\bar{b}b\bar{d}} Z_{c\bar{c}e\bar{f}} \equiv Z^{(1)}_{a\bar{d}} Z^{(2)}_{e\bar{f}}$).

condition of the second kind:

$$[\tilde{Z}^{(n)}_{a\bar{b}c\bar{d}}]^* = \tilde{Z}^{(n)}_{d\bar{c}b\bar{a}}, \qquad n = 3, 4. \tag{E13}$$

The final class of rank-four tensors involves $Z^{(n)}_{a\bar{b}}$ (for $n = 1, 2$). These are

$$Z^{(1n)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{b}c\bar{f}} Z^{(n)}_{f\bar{d}}, \qquad Z^{(5n)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{b}f\bar{d}} Z^{(n)}_{c\bar{f}}, \tag{E14}$$

$$Z^{(2n)}_{a\bar{b}c\bar{d}} \equiv Z_{c\bar{b}a\bar{f}} Z^{(n)}_{f\bar{d}}, \qquad Z^{(6n)}_{a\bar{b}c\bar{d}} \equiv Z_{c\bar{b}f\bar{d}} Z^{(n)}_{a\bar{f}}, \tag{E15}$$

$$Z^{(3n)}_{a\bar{b}c\bar{d}} \equiv Z_{c\bar{d}a\bar{f}} Z^{(n)}_{f\bar{b}}, \qquad Z^{(7n)}_{a\bar{b}c\bar{d}} \equiv Z_{c\bar{d}f\bar{b}} Z^{(n)}_{a\bar{f}}, \tag{E16}$$

$$Z^{(4n)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{d}c\bar{f}} Z^{(n)}_{f\bar{b}}, \qquad Z^{(8n)}_{a\bar{b}c\bar{d}} \equiv Z_{a\bar{d}f\bar{b}} Z^{(n)}_{c\bar{f}}. \tag{E17}$$

These tensors possess neither the Hermiticity nor the symmetry properties of $Z_{a\bar{b}c\bar{d}}$. Instead, we have (for $n = 1, 2$)

$$[Z^{(mn)}_{a\bar{b}c\bar{d}}]^* = Z^{(m+4,n)}_{b\bar{a}d\bar{c}}, \qquad m = 1, \ldots, 4. \tag{E18}$$

Note that $Z^{(2n)}_{a\bar{b}c\bar{d}} \equiv Z^{(1n)}_{c\bar{b}a\bar{d}}$, $Z^{(3n)}_{a\bar{b}c\bar{d}} \equiv Z^{(1n)}_{c\bar{d}a\bar{b}}$, and $Z^{(4n)}_{a\bar{b}c\bar{d}} \equiv Z^{(1n)}_{a\bar{d}c\bar{b}}$ are all distinct due to the lack of symmetry under the interchange of indices.

We proceed to examine all possible quadratic and cubic scalar Z-invariants. The quadratic scalar Z-invariants are obtained by summing over the indices of the tensors defined above in all possible allowed ways. However, note that the two-index tensors are Hermitian, and any four-index tensor summed over two indices yields a two-index Hermitian tensor. Hence any quadratic Z-invariant is the trace of a Hermitian tensor and is hence real. We thus turn to the (nontrivial) cubic Z-invariants. These must be of the form $Z^{(n)}_{a\bar{b}} X_{b\bar{a}}$ ($n = 1$ or 2) where $X_{b\bar{a}}$ is one of the quadratic second-rank tensors defined above, or of the form $Z_{a\bar{b}c\bar{d}} X_{b\bar{a}d\bar{c}}$, where $X_{b\bar{a}d\bar{c}}$ is one of the quadratic fourth-rank tensors defined above. But, for any Hermitian second-rank tensor, $X_{b\bar{a}}$, the quantity $Z^{(n)}_{a\bar{b}} X_{b\bar{a}}$ is real. Similarly, for any fourth-rank tensor $X_{b\bar{a}d\bar{c}}$ that either satisfies the Hermiticity conditions of the first or second kind [see Eqs. (E12) and (E13)], the quantity $Z_{a\bar{b}c\bar{d}} X_{b\bar{a}d\bar{c}}$ is real. All that remains is to check that the scalar quantities of the form $Z_{a\bar{b}c\bar{d}} Z^{(mn)}_{b\bar{a}d\bar{c}}$ are real. This is proved by first establishing the following nontrivial result:

$$Z_{a\bar{b}c\bar{d}} Z^{(mn)}_{b\bar{a}d\bar{c}} = Z_{a\bar{b}c\bar{d}} Z^{(m+4,n)}_{b\bar{a}d\bar{c}}. \tag{E19}$$

We have checked this result explicitly with MATHEMATICA (although a simple analytic proof eludes us). Using Eq. (E18), it immediately follows that all such Z-invariants are real. This completes the proof that all cubic Z-invariants are real.

We next turn to the scalar invariants that are linear in Y. Since for any Hermitian two-index tensor $X_{b\bar{a}}$, the quantity $Y_{a\bar{b}} X_{b\bar{a}}$ is real, it immediately follows that any scalar invariant that is linear in Y and at most quadratic in the Z's is real. Finally, consider scalar invariants that are quadratic in the Y's. Note that $Y_{a\bar{b}} Y_{c\bar{d}}$ has the same Hermiticity property as $Z_{a\bar{b}c\bar{d}}$, and $Y_{a\bar{c}} Y_{c\bar{b}}$ is a Hermitian two-index tensor. Thus, any scalar invariant quadratic in the Y's and linear in Z is real. Hence, we have proven that all cubic invariants are real.

It is instructive to see where the above arguments break down when quartic invariants are considered. The simplest complex scalar invariant that is linear in Y is at least cubic in Z. Indeed,

$$I_{Y3Z} = \mathrm{Im}(Z^{(1)}_{a\bar{c}} Z^{(11)}_{c\bar{d}} Y_{d\bar{a}}) = \mathrm{Im}[\mathrm{Tr}(Z^{(1)} Z^{(11)} Y)] \tag{E20}$$

is a potentially complex quartic invariant. Note that although Y, $Z^{(1)}$ and $Z^{(11)}$ are all Hermitian 2×2 matrices, I_{Y3Z} is not necessarily real because $Z^{(1)}$ and $Z^{(11)}$ do not commute. More generally, one can check that all manifestly complex scalar invariants that are linear in Y and cubic in Z can be written in the form $\mathrm{Tr}(Z^{(n)} Z^{(pq)} Y)$ or $\mathrm{Tr}(Z^{(pq)} Z^{(n)} Y)$. A simple MATHEMATICA computation reveals that

$$I_{Y3Z} = \mathrm{Im}(Z^{(n)}_{a\bar{c}} Z^{(pq)}_{c\bar{d}} Y_{d\bar{a}}) = -\mathrm{Im}(Z^{(pq)}_{c\bar{d}} Z^{(n)}_{a\bar{c}} Y_{d\bar{a}}) \tag{E21}$$

for all possible values of $n, q = 1, 2$ and $p = 1, 2, 3$. The last equality in Eq. (E21) follows from the Hermiticity of the $Z^{(n)}$, $Z^{(pq)}$ and Y. Hence, we conclude that the imaginary parts of all complex invariants of this type are equal to $\pm I_{Y3Z}$.

The simplest complex scalar invariant that is quadratic in Y is at least quadratic in Z. Indeed,

$$I_{2Y2Z} = \mathrm{Im}(Y_{a\bar{b}} Y_{c\bar{d}} Z^{(11)}_{b\bar{a}d\bar{c}}) \tag{E22}$$

is a potentially complex quartic invariant. This quantity is not necessarily real since $Z^{(11)}_{b\bar{a}d\bar{c}}$ does not satisfy any Hermiticity conditions. More generally, one can check that all manifestly complex scalar invariants that are quadratic in both Y and Z can be written in the form $Y_{a\bar{b}} Y_{c\bar{d}} Z^{(mn)}_{b\bar{a}d\bar{c}}$ (for $m = 1, \ldots, 8$ and $n = 1, 2$).[31] A simple MATHEMATICA computation reveals that

$$I_{2Y2Z} = \mathrm{Im}(Y_{a\bar{b}} Y_{c\bar{d}} Z^{(mn)}_{b\bar{a}d\bar{c}}) = -\mathrm{Im}(Y_{a\bar{b}} Y_{c\bar{d}} Z^{(m+4,n)}_{b\bar{a}d\bar{c}}) \tag{E23}$$

for all possible values of $m = 1, \ldots, 4$ and $n = 1, 2$ [where the second equality above is a consequence of Eq. (E18)]. Hence, we conclude that the imaginary parts of all complex invariants of this type are equal to $\pm I_{2Y2Z}$.

Finally, a comprehensive analytic study of nth-order pure Z-invariants for $n \geq 4$ of the type employed above (in the analysis of the cubic invariants) seems prohibitive. Thus, a systematic MATHEMATICA-aided study was carried

[31] In particular, it is straightforward to show that $Y_{a\bar{b}} Y_{c\bar{d}} Z^{(n)}_{b\bar{a}d\bar{c}}$ and $Y_{a\bar{b}} Y_{c\bar{d}} \tilde{Z}^{(n)}_{b\bar{a}d\bar{c}}$ are real due to the Hermiticity properties of Y, $Z^{(n)}$ and $\tilde{Z}^{(n)}$.

out to prove that all fourth- and fifth-order Z-invariants are real.

APPENDIX F: TIME-REVERSAL INVARIANCE OF THE HIGGS VACUUM

In this Appendix, we assume that the Higgs scalar action is explicitly CP conserving (and hence time-reversal invariant by the CPT theorem). That is, there exists a time-reversal operator $\mathcal{T}$ that satisfies Eq. (A2) (for some choice of U_T). In this context, we ask whether the Higgs *vacuum* is time-reversal invariant. However, there is an apparent ambiguity, since as shown in Appendix A there may be a number of distinct choices for the time-reversal operator (under which the action is invariant). This ambiguity corresponds to a nontrivial discrete group $\mathcal{D}$ that is a symmetry of the scalar Lagrangian. In general, the vacuum is *not* invariant with respect to $\mathcal{D}$. In this case, the vacuum may select one distinct choice for the time-reversal operator. We shall denote this choice below by $\mathcal{T}$. That is, the *theory* is time-reversal invariant if the Higgs scalar action is CP conserving and the vacuum is invariant with respect to (at least) one of the distinct choices for the time-reversal operator. If there is no choice for the time-reversal operator such that the vacuum is invariant, then time-reversal invariance is spontaneously broken.

We denote the vacuum state by $|0\rangle$ and define $\Phi_a|0\rangle \equiv |\Phi\rangle$. The action of the time-reversal operator is denoted by

$$\mathcal{T}|0\rangle \equiv |0_T\rangle, \qquad \mathcal{T}|\Phi\rangle \equiv |\Phi_T\rangle. \tag{F1}$$

The antiunitarity of $\mathcal{T}$ implies that $\langle 0_T \mid \Phi_T\rangle = \langle 0 \mid \Phi\rangle^*$. Invariance of the vacuum under time-reversal invariance implies that $|0\rangle = |0_T\rangle$. Hence $\langle 0 \mid \Phi_T\rangle = \langle 0 \mid \Phi\rangle^*$. It then follows that

$$\langle 0|\mathcal{T}\Phi_a\mathcal{T}^{-1}|0\rangle = \langle 0|\Phi_a|0\rangle^*, \tag{F2}$$

after inserting $\mathcal{T}\mathcal{T}^{-1}$ in the appropriate spot and using $\mathcal{T}|0\rangle = |0\rangle$. Using Eq. (A1), we end up with [19]:

$$(U_T)_{a\bar{b}}\langle\Phi_b\rangle = \langle\Phi_a\rangle^*, \tag{F3}$$

where $\langle\Phi_a\rangle \equiv \langle 0|\Phi_a|0\rangle$. We can use the above results to prove Theorem 3 of Sec. V.

Theorem 3.—Given an explicitly CP-conserving Higgs potential, the vacuum is time-reversal invariant if and only if a real basis exists in which the Higgs vacuum expectation values are real.

We prove this theorem by demonstrating that Eq. (F3) provides the real basis in which the vacuum expectation values are real. By assumption, Eq. (F3) is satisfied in the Φ-basis (which may or may not be a real basis). As shown in Appendix B, one can always write $U_T = V^TV$, where the unitary matrix V is unique up to multiplication on the left by an arbitrary orthogonal matrix. Inserting this result into Eq. (F3) yields

$$V\langle\Phi\rangle = [V\langle\Phi\rangle]^*, \tag{F4}$$

which implies that the vacuum expectation values are real in the Φ'-basis, where $\Phi' \equiv V\Phi$. However, Eqs. (A8) and (A11) imply that the Φ'-basis is a real basis. Of course, if the vacuum expectation values are real in a basis in which all the Higgs potential parameters are real, then the choice $U_T = I$ in Eq. (A1) yields a viable time-reversal operator. Conversely, if the Higgs scalar action is time-reversal invariant but no real basis exists in which the vacuum expectation values are real, then no viable time-reversal transformation law exists. In particular, no choice of U_T exists that satisfies Eq. (F3). This can only imply that $\mathcal{T}|0\rangle \neq |0\rangle$. In this case, the time-reversal symmetry is spontaneously broken. Thus, Theorem 3 is proven.

The conditions for a time-reversal invariant theory can therefore be reformulated. The scalar sector of the theory is time-reversal invariant if a U_T exists that satisfies Eqs. (A2) and (F3). In practice, the existence or nonexistence of such a U_T may be difficult to discern, whereas the corresponding basis-independent conditions quoted in Sec. V are straightforward to implement.

Note that the existence of real bases does not necessarily imply that the vacuum expectation values are real in *all* possible real basis choices. In Appendix A, we demonstrated that if the scalar action is time-reversal invariant then different choices for $\mathcal{T}$ correspond to different real bases in which $U_T = I$. If the time-reversal operator is defined according to Eq. (A1) then $U_T = V^TV$ yields a real basis $\Phi' = V\Phi$ in which $U'_T = I$. Alternatively, if the time-reversal operator is defined according to Eq. (A12), then $\tilde{U}_T = \tilde{V}^T\tilde{V}$ yields a real basis $\Phi'' = \tilde{V}\Phi$ in which $\tilde{U}''_T = I$. The transformation between these two real bases is $\Phi'' = W\Phi'$, where W spans an $O(2) \times \mathcal{D}$ subgroup of U(2).[32] In Appendix A, we noted that $U''_T = (WW^T)^{-1}$ and $\tilde{U}'_T = W^TW$. If $\mathcal{D}$ is trivial, then $WW^T = W^TW = I$ and $U_T = I$ (up to an overall phase) in *any* real basis. Equation (F3) then implies that the vacuum expectation values are relatively real in any real basis [and can be chosen real with an appropriate $U(1)_Y$ phase rotation]. If $\mathcal{D}$ is nontrivial, then the vacuum expectation values cannot be relatively real in both the Φ'-basis and the Φ''-basis if $\Phi'' = W\Phi'$, where $WW^T \neq e^{i\eta}I$.

As a simple example, consider again the model specified by Eq. (36) with λ_6 real, which was examined at the end of Sec. V. The Φ-basis in this case is a real basis but the vacuum expectation values, $\sqrt{2}\hat{v} = (e^{-i\xi/2}, e^{i\xi/2})$, exhibit a nontrivial relative phase for $\xi \neq 0 \pmod{\pi}$. Nevertheless, the Higgs vacuum is time-reversal invariant. In this case, we can explicitly exhibit the matrix U_T that satisfies Eq. (F3) and a unitary matrix V such that $U_T = V^TV$:

[32] One can also perform a $U(1)_Y$ transformation, which does not modify the relative phase of the two vacuum expectation values.

$$U_T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad V = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}, \quad \text{(F5)}$$

where θ is an arbitrary angle. Indeed, the matrix V transforms the (real) Φ-basis to another real basis in which the vacuum expectation values are real. In particular, the choice of $\theta = \xi/2$ yields $\hat{v}' = V\hat{v} = (1, 0)$ as noted at the end of Sec. V.

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