

Basis-independent treatment of the complex 2HDM

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The complex 2HDM (C2HDM) is the most general CP-violating two Higgs-doublet-model that possesses a softly broken \mathbb{Z}_2 symmetry. However, the physical consequences of the model cannot depend on the basis of scalar fields used to define it. Thus, to get a better sense of the significance of the C2HDM parameters, we have analyzed this model by employing a basis-independent formalism. This formalism involves transforming to the Higgs basis (which is defined up to an arbitrary complex phase) and identifying quantities that are invariant with respect to this phase degree of freedom. Using this method, we have obtained the constraints that enforce the softly broken \mathbb{Z}_2 symmetry. One can then relate the C2HDM parameters to basis-independent quantities up to a twofold ambiguity. We then show how this remaining ambiguity is resolved. We also examine the possibility of spontaneous CP violation when the scalar potential of the C2HDM is explicitly CP conserving. Basis-independent constraints are presented that govern the presence of spontaneous CP violation.

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I. INTRODUCTION

The two-Higgs-doublet model (2HDM) is one of the most well-studied extensions of the Standard Model (SM). Various motivations for adding a second hypercharge-one complex Higgs doublet to the Standard Model have been advocated in the literature [1–12]. In most cases, the structure of the 2HDM scalar potential is constrained in some way. For example, many papers assume a CP-conserving scalar potential and vacuum in order to simplify the resulting Higgs phenomenology. In such models, the three neutral Higgs bosons are states of definite CP, consisting of two CP-even scalars and one CP-odd scalar.

The assumption of CP conservation in the bosonic sector of the 2HDM may not be tenable in light of the CP-violating effects that necessarily exist in the Higgs-fermion Yukawa couplings [which are the source of the phase of the Cabibbo-Kobayashi-Maskawa (CKM) matrix that governs flavor physics]. However, the most general 2HDM scalar potential and Yukawa couplings generically yield

Higgs-mediated flavor-changing neutral currents (FCNCs) at tree level in conflict with experimental observations (which imply that FCNCs are significantly suppressed). The simplest way to avoid tree-level Higgs-mediated FCNCs is to impose a discrete \mathbb{Z}_2 symmetry on the Higgs Lagrangian [13–15]. Remarkably, such a symmetry, if exact, removes tree-level Higgs-mediated FCNCs in the Yukawa sector while eliminating all CP-violating phases in the bosonic sector of the theory. However, the imposition of an exact \mathbb{Z}_2 symmetry is too restrictive. For example, no decoupling limit exists in the \mathbb{Z}_2 -symmetric 2HDM [16]. Since the LHC Higgs data imply that the observed Higgs boson is SM-like in its properties, one can only achieve approximate Higgs alignment without decoupling by a fine-tuning of the Higgs scalar potential parameters [16–23].

It is possible to satisfy the phenomenological constraint of suppressed Higgs-mediated FCNCs by introducing a soft breaking of the \mathbb{Z}_2 symmetry. Having introduced such a symmetry breaking term in the Higgs Lagrangian, it is now possible that unremovable complex phases in the scalar potential exist, in which case Higgs-mediated CP-violating effects will be present. The 2HDM with a softly broken \mathbb{Z}_2 symmetry and unremovable complex phases in the scalar potential is called the complex 2HDM (often denoted as the C2HDM) [24–32].

The C2HDM is typically exhibited in a scalar field basis in which the \mathbb{Z}_2 symmetry of the dimension-four terms of the Higgs Lagrangian is manifest. Nevertheless, the physical consequences of the C2HDM are independent of the choice of basis. It is often convenient to employ a

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basis-independent formalism [33], in which the relevant parameters of the model are manifestly independent of the basis choice. Indeed, basis-independent couplings (in principle) can always be directly related to physical observables. Thus, it is useful to express the parameters of the C2HDM, defined in the basis in which the \mathbb{Z}_2 symmetry is manifestly realized, in terms of basis-independent quantities.

To see utility of the basis-independent approach, consider the well-known quantity,

$$\tan\beta \equiv \frac{|\langle\Phi_2^0\rangle|}{|\langle\Phi_1^0\rangle|}, \quad (1)$$

given by the ratio of the absolute values of the two neutral Higgs field vacuum expectation values defined in some basis of the scalar fields. In the most general 2HDM, this quantity is basis dependent and thus no physical observable can depend on it. In the C2HDM, $\tan\beta$ is defined via the Higgs-fermion Yukawa couplings in a basis where the \mathbb{Z}_2 symmetry of the dimension-four terms of the Higgs Lagrangian is manifestly realized. However, even given such a definition, some residual basis dependence remains. Moreover, no coupling in the bosonic sector of the C2HDM depends on $\tan\beta$ [34].

In this paper, we follow the basis-independent formalism of Refs. [33,34], which was inspired by an elegant formulation of the 2HDM in Ref. [8] that was subsequently described in more detail in Ref. [9]. An alternative approach to basis-independent methods in the 2HDM based on employing a set of independent physical couplings is given in Refs. [31,35]. The translation between these two approaches can be found in Appendix D of Ref. [23]. The bilinear formalism of the 2HDM employed in Refs. [36–41] also provides a powerful framework for establishing basis-independent results that can be applied in numerous applications.

In order to make this paper self-contained, we recapitulate in Sec. II the ingredients of the basis-independent treatment of the 2HDM developed in Refs. [33,34] in full detail. In particular, we emphasize the singular importance of the Higgs basis (defined to be a basis in which one of the two neutral scalar fields has zero vacuum expectation value), which possesses some important invariant features. In this regard, we tweak the formalism of Ref. [34] to emphasize the significance of the complex phase degree of freedom associated with the definition of the Higgs basis. This allows us to define *invariant* Higgs basis scalar fields, which simplifies the subsequent analysis.

In Sec. III, we obtain expressions for the charged and neutral Higgs mass-eigenstate fields in terms of the invariant Higgs basis fields, which can then be expressed in terms of the scalar fields of the original basis. The neutral Higgs mass eigenstates arise after the diagonalization of a 3×3 squared-mass matrix, which yields three invariant mixing angles. Although we have slightly modified the

formalism of Ref. [34], we can explicitly show that one invariant mixing angle combines additively with a parameter that represents the phase dependence implicit in the definition of the Higgs basis. Hence, only two of the three invariant mixing angles can be related to physical observables.

In Sec. IV, we introduce a basis-invariant description of the Higgs-fermion Yukawa interactions. We again tweak the formalism of Ref. [34] in order to construct matrix invariant Yukawa couplings. We then introduce the Type-I and Type-II Yukawa Higgs-quark couplings [42–44] by imposing a (softly broken) \mathbb{Z}_2 symmetry that defines the parameter $\tan\beta$ and guarantees the absence of tree-level Higgs-mediated FCNCs. Although the physics literature treats $\tan\beta$ as a physical parameter of the 2HDM,¹ we emphasize that a residual basis dependence is still present and associated with the freedom to interchange the two Higgs fields in a basis where the softly broken \mathbb{Z}_2 symmetry is manifestly realized.

In Sec. V, a basis-independent treatment of the softly broken \mathbb{Z}_2 symmetry (which is needed in the construction of the Type-I and Type-II Yukawa interactions) is presented. Formal basis-independent expressions were originally given in Ref. [33], and explicit results in the case of the CP-conserving 2HDM were presented in Ref. [45]. In this paper, we provide the corresponding results that are applicable if CP violation is present in the 2HDM, with a careful analysis of all possible special cases. We subsequently noticed that some equivalent results can also be found in a paper by Lavoura [46], although the basis-independent nature of Lavoura’s results was not initially appreciated.

In Sec. VI, we are finally ready to carry out the basis-independent treatment of the C2HDM. In the literature, the parameters of the C2HDM are typically defined in the basis where the softly broken \mathbb{Z}_2 symmetry is manifest and where the two scalar field vacuum expectation values are real and positive. Our goal was to provide a translation between these parameters and the corresponding parameters of the basis-independent formalism. In doing so, one gains insight into the nature of the original C2HDM parameters and their relations to physical quantities. We again emphasize the significance of the residual basis dependence associated with the interchange of the two scalar fields.

In Sec. VII, we return to the paper of Lavoura [46]. We provide the necessary detail to derive Lavoura’s results and indicate where his results fall short (i.e., special cases

¹The definition of the term “physical parameter” requires some care. In this paper, we identify a Lagrangian parameter as a physical parameter if it can be uniquely related to quantities that can be obtained (in principle) from direct experimental measurements. Note that parameters that cannot be defined in terms of quantities that are invariant with respect to field redefinitions are not physical parameters.

in which Lavoura's results do not apply). Lavoura attempted to find two invariant conditions for identifying the presence of spontaneous CP violation in the 2HDM. He was able to find one of the conditions but unable to find the second one. We complete his search and discuss various special cases in which only one invariant condition is required.

We briefly summarize our conclusions in Sec. VIII. Additional details are relegated to five appendices. Appendix A provides the necessary formulae for transforming between two scalar field bases. In particular, we exhibit how the parameters of the original basis of the 2HDM are expressed in terms of the parameters of the Higgs basis. Appendix B treats the so-called exceptional region of the 2HDM parameter space (the nomenclature was introduced in Ref. [47]). Indeed, in this parameter regime, special attention is mandated as some of our derivations of basis-independent conditions provided in the main text are not applicable in this case. Appendix C

demonstrates that the formal basis-independent conditions for a (softly broken) \mathbb{Z}_2 symmetry given in Ref. [33] are equivalent to the results of the explicit derivation given in Sec. V. Appendix D provides a simple proof for the existence of a particular basis of scalar field in which the CP-odd invariants employed in Sec. VII take on especially convenient forms. Finally, Appendix E examines the mixing of the three neutral physical scalars of the 2HDM in a generic basis of the two scalar fields.

II. BASIS-INDEPENDENT FORMALISM OF THE 2HDM

The fields of the two-Higgs-doublet model (2HDM) consist of two identical complex hypercharge one, SU(2) doublet scalar fields $\Phi_a(x) \equiv (\Phi_a^+(x), \Phi_a^0(x))$, where the ‘‘Higgs flavor’’ index $a = 1, 2$ labels the two-Higgs-doublet fields. The most general renormalizable SU(2)_L × U(1)_Y invariant scalar potential is given by

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

where m_{11}^2, m_{22}^2 , and $\lambda_1, \dots, \lambda_4$ are real parameters and $m_{12}^2, \lambda_5, \lambda_6$ 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 U(1)_{EM} gauge symmetry. Then, the scalar field vacuum expectations values (vevs) are of the form

$$\langle \Phi_1 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \quad \langle \Phi_2 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v_2 e^{i\xi} \end{pmatrix}, \quad (3)$$

where v_1 and v_2 are real and non-negative, $0 \leq \xi < 2\pi$, and v is determined by the Fermi constant,

$$v \equiv (v_1^2 + v_2^2)^{1/2} = \frac{2m_W}{g} = (\sqrt{2}G_F)^{-1/2} = 246 \text{ GeV}. \quad (4)$$

In writing Eq. (3), we have used a global U(1)_Y hypercharge transformation to eliminate the phase of v_1 . The bosonic part of the Higgs Lagrangian consists of a sum of the scalar potential [Eq. (2)] and the gauge invariant kinetic energy term,

$$\mathcal{L}_{\text{KE}} = (D_\mu \Phi)_a^\dagger (D^\mu \Phi)_a. \quad (5)$$

In Eq. (5), the covariant derivative of the electroweak gauge group acting on the scalar fields yields

$$D_\mu \Phi_a = \begin{pmatrix} \partial_\mu \Phi_a^+ + \left[\frac{ig}{c_W} \left(\frac{1}{2} - s_W^2 \right) Z_\mu + ieA_\mu \right] \Phi_a^+ + \frac{ig}{\sqrt{2}} W_\mu^+ \Phi_a^0 \\ \partial_\mu \Phi_a^0 - \frac{ig}{2c_W} Z_\mu \Phi_a^0 + \frac{ig}{\sqrt{2}} W_\mu^- \Phi_a^+ \end{pmatrix}, \quad (6)$$

where $s_W \equiv \sin \theta_W$ and $c_W \equiv \cos \theta_W$.

Since the scalar doublets Φ_1 and Φ_2 have identical SU(2) × U(1) quantum numbers, one is free to express the scalar potential in terms of two orthonormal linear combinations of the original scalar fields. The parameters appearing in Eq. (2) depend on a particular *basis choice* of the two scalar fields (denoted henceforth as the Φ basis). The most general redefinition of the scalar fields that leaves \mathcal{L}_{KE} invariant corresponds to a global U(2) transformation, $\Phi_a \rightarrow U_{a\bar{b}} \Phi_b$ [and $\Phi_a^\dagger \rightarrow \Phi_b^\dagger U_{b\bar{a}}^\dagger$], where the 2×2 unitary matrix U satisfies $U_{b\bar{a}}^\dagger U_{a\bar{c}} = \delta_{b\bar{c}}$. In our convention of employing unbarred and barred indices, there is an implicit sum over unbarred–barred index pairs such as a and \bar{a} .²

Following Refs. [8,9,33], the scalar potential can be written in U(2)-covariant form,

²Note that replacing an unbarred index with a barred index is equivalent to complex conjugation. An alternative but equivalent convention makes use of lower and upper Higgs flavor indices in place of barred and unbarred indices, in which case there is an implicit sum over a repeated upper-lower index pair.

$$\mathcal{V} = Y_{a\bar{b}}\Phi_a^\dagger\Phi_b + \frac{1}{2}Z_{a\bar{b}c\bar{d}}(\Phi_a^\dagger\Phi_b)(\Phi_c^\dagger\Phi_d), \quad (7)$$

where the quartic couplings satisfy $Z_{a\bar{b}c\bar{d}} = Z_{c\bar{d}a\bar{b}}$. The hermiticity of the scalar potential implies that $Y_{a\bar{b}} = (Y_{b\bar{a}})^*$ and $Z_{a\bar{b}c\bar{d}} = (Z_{b\bar{a}d\bar{c}})^*$. Under a flavor-U(2) transformation, the tensors $Y_{a\bar{b}}$ and $Z_{a\bar{b}c\bar{d}}$ transform covariantly: $Y_{a\bar{b}} \rightarrow U_{a\bar{c}}Y_{c\bar{d}}U_{d\bar{b}}^\dagger$ and $Z_{a\bar{b}c\bar{d}} \rightarrow U_{a\bar{e}}U_{f\bar{b}}^\dagger U_{c\bar{g}}U_{h\bar{d}}^\dagger Z_{e\bar{f}g\bar{h}}$. The coefficients of the scalar potential depend on the choice of basis. The transformation of these coefficients under a U(2) basis change, exhibited explicitly in Eqs. (A2)–(A11), are precisely the transformation laws of Y and Z given above.

For the convenience of the reader, we recapitulate the ingredients of the basis-independent approach employed in Ref. [34], in order to make this paper self-contained. In an arbitrary scalar basis, the vevs of the two-Higgs-doublet fields [cf. Eq. (3)] can be written compactly as

$$\langle\Phi_a\rangle = \frac{v}{\sqrt{2}} \begin{pmatrix} 0 \\ \hat{v}_a \end{pmatrix}, \quad (8)$$

where $\hat{v} = (\hat{v}_1, \hat{v}_2)$ is a complex vector of unit norm. The \hat{v}_a are the nonzero solutions to the equation obtained by minimizing the scalar potential,

$$\hat{v}_a^* \left[Y_{a\bar{b}} + \frac{1}{2}v^2 Z_{a\bar{b}c\bar{d}}\hat{v}_c^*\hat{v}_d \right] = 0. \quad (9)$$

A second unit vector \hat{w} can be defined that is orthogonal to \hat{v} ,

$$\hat{w}_b = \hat{v}_a^* \epsilon_{ab}, \quad (10)$$

where $\epsilon_{12} = -\epsilon_{21} = 1$ and $\epsilon_{11} = \epsilon_{22} = 0$. Indeed, \hat{v} and \hat{w} are orthogonal due to the vanishing of the complex dot product, $\hat{v}_b^*\hat{w}_b = 0$. Note that under a U(2) transformation,

$$\hat{v}_a \rightarrow U_{a\bar{b}}\hat{v}_b, \quad \text{which implies that } \hat{w}_a \rightarrow (\det U)^{-1}U_{a\bar{b}}\hat{w}_b. \quad (11)$$

Since the tensors $Y_{a\bar{b}}$ and $Z_{a\bar{b}c\bar{d}}$ exhibit tensorial properties with respect to global U(2) transformations in the Higgs flavor space, one can easily construct invariants with respect to the U(2) by forming U(2)-scalar quantities. It is convenient to define two Hermitian projection operators,

$$V_{a\bar{b}} \equiv \hat{v}_a\hat{v}_b^*, \quad W_{a\bar{b}} \equiv \hat{w}_a\hat{w}_b^* = \delta_{a\bar{b}} - V_{a\bar{b}}. \quad (12)$$

The matrices V and W can be used to define the following manifestly basis-invariant real quantities that depend on the scalar potential parameters [cf. Eq. (7)]:

$$Y_1 \equiv \text{Tr}(YV), \quad Y_2 \equiv \text{Tr}(YW), \quad (13)$$

$$Z_1 \equiv Z_{a\bar{b}c\bar{d}}V_{b\bar{a}}V_{d\bar{c}}, \quad Z_2 \equiv Z_{a\bar{b}c\bar{d}}W_{b\bar{a}}W_{d\bar{c}}, \quad (14)$$

$$Z_3 \equiv Z_{a\bar{b}c\bar{d}}V_{b\bar{a}}W_{d\bar{c}}, \quad Z_4 \equiv Z_{a\bar{b}c\bar{d}}V_{b\bar{c}}W_{d\bar{a}}. \quad (15)$$

In addition, we shall define the following pseudoinvariant (potentially complex) quantities:

$$Y_3 \equiv Y_{a\bar{b}}\hat{v}_a^*\hat{w}_b, \quad (16)$$

$$Z_5 \equiv Z_{a\bar{b}c\bar{d}}\hat{v}_a^*\hat{w}_b\hat{v}_c^*\hat{w}_d, \quad (17)$$

$$Z_6 \equiv Z_{a\bar{b}c\bar{d}}\hat{v}_a^*\hat{v}_b\hat{v}_c^*\hat{w}_d, \quad (18)$$

$$Z_7 \equiv Z_{a\bar{b}c\bar{d}}\hat{v}_a^*\hat{w}_b\hat{w}_c^*\hat{w}_d. \quad (19)$$

In particular, Eq. (11) implies that under a basis transformation, $\Phi_a \rightarrow U_{a\bar{b}}\Phi_b$,

$$[Y_3, Z_6, Z_7] \rightarrow (\det U)^{-1}[Y_3, Z_6, Z_7] \quad \text{and} \\ Z_5 \rightarrow (\det U)^{-2}Z_5. \quad (20)$$

Note that $Z_5^*Z_6^2$, $Z_5^*Z_7^2$, and $Z_6^*Z_7$ are basis-invariant quantities that can be obtained from the pseudoinvariants Z_5 , Z_6 , and Z_7 .

Once the scalar potential minimum is determined, which defines \hat{v}_a , one can introduce new Higgs-doublet fields that define the Higgs basis,

$$H_1 = (H_1^+, H_1^0) \equiv \hat{v}_a^*\Phi_a, \quad H_2 = (H_2^+, H_2^0) \equiv \hat{w}_a^*\Phi_a. \quad (21)$$

The definitions of H_1 and H_2 imply that

$$\langle H_1^0 \rangle = \frac{v}{\sqrt{2}}, \quad \langle H_2^0 \rangle = 0, \quad (22)$$

where we have used Eq. (8) and the fact that \hat{v} and \hat{w} are complex orthogonal unit vectors. Note that the definition of the scalar field H_1 is basis independent, whereas the scalar field H_2 is a pseudoinvariant field due to the transformation properties of \hat{w} given in Eq. (11). That is, $H_2 \rightarrow (\det U)H_2$ under $\Phi_a \rightarrow U_{a\bar{b}}\Phi_b$, where $\det U$ is a pure phase. The pseudoinvariant nature of H_2 is ultimately due to the fact that one can rephase H_2 while maintaining Eq. (22) which defines the Higgs basis. Thus, one should really speak of a class of Higgs bases that is characterized by an arbitrary phase angle.

The significance of the quantities defined by Eqs. (13)–(19) becomes clearer after rewriting the scalar potential in terms of the Higgs basis fields,

$$\begin{aligned}
\mathcal{V} = & Y_1 H_1^\dagger H_1 + Y_2 H_2^\dagger H_2 + [Y_3 H_1^\dagger H_2 + \text{H.c.}] \\
& + \frac{1}{2} Z_1 (H_1^\dagger H_1)^2 + \frac{1}{2} Z_2 (H_2^\dagger H_2)^2 + Z_3 (H_1^\dagger H_1)(H_2^\dagger H_2) + Z_4 (H_1^\dagger H_2)(H_2^\dagger H_1) \\
& + \left\{ \frac{1}{2} Z_5 (H_1^\dagger H_2)^2 + [Z_6 (H_1^\dagger H_1) + Z_7 (H_2^\dagger H_2)] H_1^\dagger H_2 + \text{H.c.} \right\}. \tag{23}
\end{aligned}$$

The minimization of the scalar potential in the Higgs basis yields

$$Y_1 = -\frac{1}{2} Z_1 v^2, \quad Y_3 = -\frac{1}{2} Z_6 v^2. \tag{24}$$

In light of Eq. (20), the form of the scalar potential is invariant under the rephasing of the pseudoinvariant Higgs basis field H_2 . However, one can make the basis invariance of the scalar potential even more explicit by introducing invariant Higgs basis fields,

$$\mathcal{H}_1 \equiv H_1, \quad \mathcal{H}_2 \equiv e^{i\eta} H_2, \tag{25}$$

where $e^{i\eta}$ is a pseudoinvariant quantity that transforms under the basis transformation, $\Phi_a \rightarrow U_{ab} \Phi_b$ as

$$e^{-i\eta} \rightarrow (\det U) e^{-i\eta}. \tag{26}$$

Equation (25) provides a new way of exhibiting explicitly the existence of the class of Higgs bases parametrized by the phase angle η . Equivalently, one can write

$$\Phi_a = \mathcal{H}_1 \hat{v}_a + e^{-i\eta} \mathcal{H}_2 \hat{w}_a. \tag{27}$$

In terms of the invariant Higgs basis fields, the scalar potential is given by

$$\begin{aligned}
\mathcal{V} = & Y_1 \mathcal{H}_1^\dagger \mathcal{H}_1 + Y_2 \mathcal{H}_2^\dagger \mathcal{H}_2 + [Y_3 e^{-i\eta} \mathcal{H}_1^\dagger \mathcal{H}_2 + \text{H.c.}] \\
& + \frac{1}{2} Z_1 (\mathcal{H}_1^\dagger \mathcal{H}_1)^2 + \frac{1}{2} Z_2 (\mathcal{H}_2^\dagger \mathcal{H}_2)^2 + Z_3 (\mathcal{H}_1^\dagger \mathcal{H}_1)(\mathcal{H}_2^\dagger \mathcal{H}_2) + Z_4 (\mathcal{H}_1^\dagger \mathcal{H}_2)(\mathcal{H}_2^\dagger \mathcal{H}_1) \\
& + \left\{ \frac{1}{2} Z_5 e^{-2i\eta} (\mathcal{H}_1^\dagger \mathcal{H}_2)^2 + [Z_6 e^{-i\eta} (\mathcal{H}_1^\dagger \mathcal{H}_1) + Z_7 e^{-i\eta} (\mathcal{H}_2^\dagger \mathcal{H}_2)] \mathcal{H}_1^\dagger \mathcal{H}_2 + \text{H.c.} \right\}. \tag{28}
\end{aligned}$$

Due to Eqs. (20) and (26), all the coefficients of the scalar potential given in Eq. (28) are manifestly basis invariant.

It is instructive to see what happens if one transforms between two Higgs bases. That is, suppose that $\langle \Phi_1^0 \rangle = v/\sqrt{2}$ and $\langle \Phi_2^0 \rangle = 0$. To transform to another Higgs basis, one can employ the U(2) transformation $\Phi_a \rightarrow U_{ab} \Phi_b$, where $U = \text{diag}(1, e^{i\chi})$. Then, Eq. (26) implies that $\eta \rightarrow \eta - \chi$. It then follows that

$$[Y_3, Z_6, Z_7] \rightarrow e^{-i\chi} [Y_3, Z_6, Z_7] \quad \text{and} \quad Z_5 \rightarrow e^{-2i\chi} Z_5. \tag{29}$$

In contrast, Y_1 , Y_2 , and $Z_{1,2,3,4}$ are invariant when transforming between two Higgs bases.

To summarize, the class of Higgs bases corresponds to $\hat{v} = (1, 0)$ and $\hat{w} = (0, 1)$; different Higgs basis choices are parametrized by the phase angle η via $\mathcal{H}_2 = e^{i\eta} \Phi_2$ after inserting $\hat{w} = (0, 1)$ into Eq. (21). Indeed, inserting the Higgs basis values of \hat{v} and \hat{w} into Eqs. (13)–(19) and then rewriting the scalar potential [Eq. (7)] in terms of the invariant Higgs basis fields defined in Eq. (21) yields Eq. (28) as expected.

Finally, we note that the 2HDM scalar potential and vacuum are CP invariant if one can find a choice of η such

that all the coefficients of the scalar potential in Eq. (28) are real after imposing the scalar potential minimum conditions given in Eq. (24). This condition is satisfied if and only if [48] (see also Refs. [33,34])

$$\text{Im}(Z_5^* Z_6^2) = \text{Im}(Z_5^* Z_7^2) = \text{Im}(Z_6^* Z_7) = 0. \tag{30}$$

III. THE CHARGED AND NEUTRAL HIGGS MASS EIGENSTATES

To determine the Higgs mass eigenstates, one must examine the terms of the scalar potential that are quadratic in the scalar fields (after imposing the scalar potential minimum conditions and defining shifted fields with zero vevs). We have slightly tweaked the procedure that was carried out in Ref. [34], and we summarize the results here.

We parameterize the invariant Higgs basis fields \mathcal{H}_1 and \mathcal{H}_2 as follows:

$$\mathcal{H}_1 = \left(\frac{G^+}{\sqrt{2}} (v + \varphi_1^0 + iG^0) \right), \quad \mathcal{H}_2 = \left(\frac{H^+}{\sqrt{2}} (\varphi_2^0 + ia^0) \right), \tag{31}$$

where G^+ (and its Hermitian conjugate) are the charged Goldstone bosons and G^0 is the neutral Goldstone boson. The three remaining neutral fields mix, and the resulting neutral Higgs squared-mass matrix in the $\varphi_1^0\text{-}\varphi_2^0\text{-}a^0$ basis is

$$\mathcal{M}^2 = v^2 \begin{pmatrix} Z_1 & \text{Re}(Z_6 e^{-i\eta}) & -\text{Im}(Z_6 e^{-i\eta}) \\ \text{Re}(Z_6 e^{-i\eta}) & \frac{1}{2}[Z_{34} + \text{Re}(Z_5 e^{-2i\eta})] + Y_2/v^2 & -\frac{1}{2}\text{Im}(Z_5 e^{-2i\eta}) \\ -\text{Im}(Z_6 e^{-i\eta}) & -\frac{1}{2}\text{Im}(Z_5 e^{-2i\eta}) & \frac{1}{2}[Z_{34} - \text{Re}(Z_5 e^{-2i\eta})] + Y_2/v^2 \end{pmatrix}, \quad (32)$$

where $Z_{34} \equiv Z_3 + Z_4$.

The squared-mass matrix \mathcal{M}^2 is real symmetric; hence, it can be diagonalized by a special real orthogonal transformation,

$$R\mathcal{M}^2R^\top = \mathcal{M}_D^2 \equiv \text{diag}(m_1^2, m_2^2, m_3^2), \quad (33)$$

where R is a real matrix such that $RR^\top = I$, $\det R = 1$ and the m_i^2 are the eigenvalues of \mathcal{M}^2 . A convenient form for R is

$$\begin{aligned} R = R_{12}R_{13}\bar{R}_{23} &= \begin{pmatrix} c_{12} & -s_{12} & 0 \\ s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} c_{13} & 0 & -s_{13} \\ 0 & 1 & 0 \\ s_{13} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{c}_{23} & -\bar{s}_{23} \\ 0 & \bar{s}_{23} & \bar{c}_{23} \end{pmatrix} \\ &= \begin{pmatrix} c_{13}c_{12} & -s_{12}\bar{c}_{23} - c_{12}s_{13}\bar{s}_{23} & -c_{12}s_{13}\bar{c}_{23} + s_{12}\bar{s}_{23} \\ c_{13}s_{12} & c_{12}\bar{c}_{23} - s_{12}s_{13}\bar{s}_{23} & -s_{12}s_{13}\bar{c}_{23} - c_{12}\bar{s}_{23} \\ s_{13} & c_{13}\bar{s}_{23} & c_{13}\bar{c}_{23} \end{pmatrix}, \end{aligned} \quad (34)$$

where $c_{ij} \equiv \cos \theta_{ij}$ and $s_{ij} \equiv \sin \theta_{ij}$. We have written $\bar{c}_{23} \equiv \cos \bar{\theta}_{23}$ and $\bar{s}_{23} \equiv \sin \bar{\theta}_{23}$ to distinguish between the angle θ_{23} defined in Ref. [34] and the angle $\bar{\theta}_{23}$ defined above. Indeed, the angles θ_{12} , θ_{13} , and $\bar{\theta}_{23}$ defined above are all invariant quantities since they are obtained by diagonalizing \mathcal{M}^2 whose matrix elements are manifestly basis invariant.

The neutral physical Higgs mass eigenstates are denoted by h_1 , h_2 , and h_3 ,

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R \begin{pmatrix} \varphi_1^0 \\ \varphi_2^0 \\ a^0 \end{pmatrix} = RW \begin{pmatrix} \sqrt{2}\text{Re } \mathcal{H}_1^0 - v \\ \mathcal{H}_2^0 \\ \mathcal{H}_2^{0\dagger} \end{pmatrix}, \quad (35)$$

which defines the unitary matrix W . A straightforward calculation yields [34]

$$RW = \begin{pmatrix} q_{11} & \frac{1}{\sqrt{2}}q_{12}^*e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{12}e^{-i\bar{\theta}_{23}} \\ q_{21} & \frac{1}{\sqrt{2}}q_{22}^*e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{22}e^{-i\bar{\theta}_{23}} \\ q_{31} & \frac{1}{\sqrt{2}}q_{32}^*e^{i\bar{\theta}_{23}} & \frac{1}{\sqrt{2}}q_{32}e^{-i\bar{\theta}_{23}} \end{pmatrix}, \quad (36)$$

where the $q_{k\ell}$ are listed in Table I. Employing Eqs. (21) and (35), it follows that

$$\begin{aligned} h_k &= \frac{1}{\sqrt{2}}[\bar{\Phi}_a^{0\dagger}(q_{k1}\hat{v}_a + q_{k2}\hat{w}_a e^{-i\theta_{23}}) \\ &\quad + (q_{k1}^*\hat{v}_a^* + q_{k2}^*\hat{w}_a^* e^{i\theta_{23}})\bar{\Phi}_a^0], \end{aligned} \quad (37)$$

for $k = 1, 2, 3$, where the shifted neutral fields are defined by $\bar{\Phi}_a^0 \equiv \Phi_a^0 - v\hat{v}_a/\sqrt{2}$. It is straightforward to verify that Eq. (37) also applies to the neutral Goldstone boson if we denote $h_0 \equiv G^0$ and define $q_{01} = i$ and $q_{02} = 0$ as indicated in Table I.

We have also introduced the quantity,³

$$\theta_{23} \equiv \bar{\theta}_{23} + \eta. \quad (38)$$

Note that $e^{-i\theta_{23}}$ is a pseudoinvariant quantity. In particular, in light of Eq. (26), it follows that

$$e^{-i\theta_{23}} \rightarrow (\det U)e^{-i\theta_{23}} \quad (39)$$

under a $U(2)$ basis transformation, $\Phi_a \rightarrow U_{ab}\Phi_b$. This transformation law is consistent with Eq. (11) and the fact that the neutral Higgs mass-eigenstates h_k are invariant fields.⁴

³Note that θ_{23} corresponds precisely to the angle of the same name employed in Ref. [34].

⁴The remaining freedom to define the overall sign of h_k is associated with the convention adopted for the domains of the mixing angles θ_{ij} , as discussed in Ref. [34], and is independent of scalar field basis transformations.

TABLE I. The U(2)-invariant quantities $q_{k\ell}$ are functions of the neutral Higgs mixing angles θ_{12} and θ_{13} , where $c_{ij} \equiv \cos \theta_{ij}$ and $s_{ij} \equiv \sin \theta_{ij}$. The neutral Goldstone boson corresponds to $k = 0$.

k	q_{k1}	q_{k2}
0	i	0
1	$c_{12}c_{13}$	$-s_{12} - ic_{12}s_{13}$
2	$s_{12}c_{13}$	$c_{12} - is_{12}s_{13}$
3	s_{13}	ic_{13}

For completeness, we note that Eqs. (21) and (31) yield expressions for the massless charged Goldstone field, $G^+ = \hat{v}_a^* \Phi_a^+$, and the charged Higgs field, $H^+ = e^{i\eta} \hat{w}_a^* \Phi_a^+$, with corresponding squared mass,

$$m_{H^\pm}^2 = Y_2 + \frac{1}{2} Z_3 v^2. \quad (40)$$

Nevertheless, one is always free to rephase the charged Higgs field without affecting any observable of the model. It is convenient to rephase, $H^+ \rightarrow e^{-i\bar{\theta}_{23}} H^+$, which yields

$$H^+ = e^{i\bar{\theta}_{23}} \mathcal{H}_2^+ = e^{i\bar{\theta}_{23}} \hat{w}_a^* \Phi_a^+. \quad (41)$$

Note that this rephasing is conventional and does not alter the fact that H^+ is an invariant field with respect to scalar field basis transformations.

Finally, one can invert Eq. (37) and include the charged scalars to obtain⁵

$$\Phi_a = \left(\begin{array}{c} G^+ \hat{v}_a + H^+ e^{-i\bar{\theta}_{23}} \hat{w}_a \\ \frac{v}{\sqrt{2}} \hat{v}_a + \frac{1}{\sqrt{2}} \sum_{k=0}^3 (q_{k1} \hat{v}_a + q_{k2} e^{-i\bar{\theta}_{23}} \hat{w}_a) h_k \end{array} \right). \quad (42)$$

Although $\bar{\theta}_{23}$ is an invariant parameter, it has no physical significance, since it only appears in Eq. (42) in the combination defined in Eq. (38). Indeed, if we now insert Eq. (42) into the expression for the scalar potential given in Eq. (7) to derive the bosonic couplings of the 2HDM, one sees that $\bar{\theta}_{23}$ never appears explicitly in any observable. Consequently, one can simply set $\bar{\theta}_{23} = 0$ without loss of generality, which would identify $\eta = \theta_{23}$ as the pseudoinvariant phase angle that specifies the choice of Higgs basis.

It is useful to rewrite the neutral Higgs mass diagonalization equation [Eq. (33)] as follows. With $R \equiv R_{12} R_{13} \bar{R}_{23}$ given by Eq. (34), we define

$$\widetilde{\mathcal{M}}^2 \equiv \bar{R}_{23} \mathcal{M}^2 \bar{R}_{23}^\dagger = v^2 \begin{pmatrix} Z_1 & \text{Re}(Z_6 e^{-i\bar{\theta}_{23}}) & -\text{Im}(Z_6 e^{-i\bar{\theta}_{23}}) \\ \text{Re}(Z_6 e^{-i\bar{\theta}_{23}}) & \text{Re}(Z_5 e^{-2i\bar{\theta}_{23}}) + A^2/v^2 & -\frac{1}{2} \text{Im}(Z_5 e^{-2i\bar{\theta}_{23}}) \\ -\text{Im}(Z_6 e^{-i\bar{\theta}_{23}}) & -\frac{1}{2} \text{Im}(Z_5 e^{-2i\bar{\theta}_{23}}) & A^2/v^2 \end{pmatrix}, \quad (43)$$

where A^2 is the auxiliary quantity,

$$A^2 \equiv Y_2 + \frac{1}{2} [Z_3 + Z_4 - \text{Re}(Z_5 e^{-2i\bar{\theta}_{23}})] v^2. \quad (44)$$

Note that we have employed Eq. (38), which results in the appearance of $e^{-i\bar{\theta}_{23}}$ in the appropriate places given that the matrix elements of $\widetilde{\mathcal{M}}^2$ are invariant quantities (but with no separate dependence on the invariant angle $\bar{\theta}_{23}$). The diagonal neutral Higgs squared-mass matrix is then given by

$$\tilde{R} \widetilde{\mathcal{M}}^2 \tilde{R}^\dagger = \mathcal{M}_D^2 = \text{diag}(m_1^2, m_2^2, m_3^2), \quad (45)$$

where the diagonalizing matrix $\tilde{R} \equiv R_{12} R_{13}$ depends only on the invariant angles θ_{12} and θ_{13} ,

$$\tilde{R} = \begin{pmatrix} c_{12}c_{13} & -s_{12} & -c_{12}s_{13} \\ c_{13}s_{12} & c_{12} & -s_{12}s_{13} \\ s_{13} & 0 & c_{13} \end{pmatrix} = \begin{pmatrix} q_{11} & \text{Re } q_{12} & \text{Im } q_{12} \\ q_{21} & \text{Re } q_{22} & \text{Im } q_{22} \\ q_{31} & \text{Re } q_{32} & \text{Im } q_{32} \end{pmatrix}. \quad (46)$$

Explicit expressions for the neutral Higgs boson squared masses requires one to solve a cubic characteristic equation that yields the eigenvalues of $\widetilde{\mathcal{M}}^2$. The resulting expressions are unwieldy and impractical. Nevertheless, one can derive useful relations by rewriting Eq. (45) as $\widetilde{\mathcal{M}}^2 = \tilde{R}^\dagger \mathcal{M}_D^2 \tilde{R}$ and employing Eq. (46). It then follows that

⁵Here we differ slightly from Ref. [34] where a noninvariant charged Higgs field, $H^+ = \hat{w}_a^* \Phi_a^+$, is employed.

$$Z_1 = \frac{1}{v^2} \sum_{k=1}^3 m_k^2 (q_{k1})^2, \quad (47)$$

$$Z_4 = \frac{1}{v^2} \left[\sum_{k=1}^3 m_k^2 |q_{k2}|^2 - 2m_{H^\pm}^2 \right], \quad (48)$$

after making use of Eq. (40) in the evaluation of Eq. (48), and

$$Z_5 e^{-2i\theta_{23}} = \frac{1}{v^2} \sum_{k=1}^3 m_k^2 (q_{k2}^*)^2, \quad (49)$$

$$Z_6 e^{-i\theta_{23}} = \frac{1}{v^2} \sum_{k=1}^3 m_k^2 q_{k1} q_{k2}^*. \quad (50)$$

The conditions for a CP-invariant scalar potential and vacuum were given in Eq. (30). These conditions are satisfied in the following two cases:

$$1. \text{Im}(Z_5 e^{-2i\theta_{23}}) = \text{Im}(Z_6 e^{-i\theta_{23}}) = \text{Im}(Z_7 e^{-i\theta_{23}}) = 0, \quad (51)$$

or

$$2. \text{Im}(Z_5 e^{-2i\theta_{23}}) = \text{Re}(Z_6 e^{-i\theta_{23}}) = \text{Re}(Z_7 e^{-i\theta_{23}}) = 0. \quad (52)$$

In both cases, the neutral scalar squared-mass matrix given in Eq. (43) assumes a block diagonal form consisting of a 2×2 mass matrix that yields the squared masses of two neutral CP-even Higgs bosons and a 1×1 mass matrix corresponding to the squared mass of a neutral CP-odd Higgs boson. In this paper, our primary focus is the 2HDM with a scalar sector that exhibits either explicit or spontaneous CP violation, in which case neither Eq. (30) nor Eqs. (51) and (52) are satisfied.

IV. HIGGS-FERMION YUKAWA INTERACTIONS

The Higgs boson couplings to the fermions arise from the Yukawa Lagrangian. We shall slightly tweak the results that were initially presented in Ref. [34] (with some corrections subsequently noted in Ref. [49]). In terms of the quark mass-eigenstate fields, the Yukawa Lagrangian in the Φ basis is given by

$$-\mathcal{L}_Y = \bar{U}_L \Phi_a^0 h_a^U U_R - \bar{D}_L K^\dagger \Phi_a^- h_a^D U_R + \bar{U}_L K \Phi_a^+ h_a^{D\dagger} D_R + \bar{D}_L \Phi_a^0 h_a^{D\dagger} D_R + \text{H.c.}, \quad (53)$$

where $Q_{R,L} \equiv P_{R,L} Q$, with $P_{R,L} \equiv \frac{1}{2}(1 \pm \gamma_5)$ [for $Q = U, D$], K is the CKM mixing matrix, and the $h^{U,D}$ are 3×3 Yukawa coupling matrices. We can construct invariant matrix Yukawa couplings κ^Q and ρ^Q by defining⁶

$$\kappa^Q \equiv \hat{v}_a^* h_a^Q, \quad \rho^Q \equiv e^{i\theta_{23}} \hat{w}_a^* h_a^Q. \quad (54)$$

Inverting these equations yields

$$h_a^Q = \kappa^Q \hat{v}_a + e^{-i\theta_{23}} \rho^Q \hat{w}_a. \quad (55)$$

Inserting the above result into Eq. (53) and employing Eqs. (21), (25), and (38), we end up with the Yukawa Lagrangian in terms of the invariant Higgs basis fields,

$$-\mathcal{L}_Y = \bar{U}_L (\kappa^U \mathcal{H}_1^{0\dagger} + e^{-i\theta_{23}} \rho^U \mathcal{H}_2^{0\dagger}) U_R - \bar{D}_L K^\dagger (\kappa^U \mathcal{H}_1^- + e^{-i\theta_{23}} \rho^U \mathcal{H}_2^-) U_R \\ + \bar{U}_L K (\kappa^{D\dagger} \mathcal{H}_1^+ + e^{i\theta_{23}} \rho^{D\dagger} \mathcal{H}_2^+) D_R + \bar{D}_L (\kappa^{D\dagger} \mathcal{H}_1^0 + e^{i\theta_{23}} \rho^{D\dagger} \mathcal{H}_2^0) D_R + \text{H.c.} \quad (56)$$

In light of Eq. (22), κ^U and κ^D are proportional to the (real non-negative) diagonal quark mass matrices M_U and M_D , respectively. In particular,

$$M_U = \frac{v}{\sqrt{2}} \kappa^U = \text{diag}(m_u, m_c, m_t), \quad M_D = \frac{v}{\sqrt{2}} \kappa^{D\dagger} = \text{diag}(m_d, m_s, m_b). \quad (57)$$

In contrast, the matrices ρ^U and ρ^D are independent complex 3×3 matrices.

⁶We have modified the definition of ρ^Q as compared to the one employed in Refs. [33,34,49] by including a factor of $e^{i\theta_{23}}$. This new definition has been adopted as a matter of convenience since ρ^Q defined as in Eq. (54) is invariant with respect to basis transformations of the scalar fields.

One can now reexpress the Higgs basis fields in terms of mass-eigenstate charged and neutral Higgs fields by inverting Eq. (35) and employing Eq. (41) to obtain the Yukawa couplings of the quarks to the physical scalars and to the Goldstone bosons. Of course, the same result can be obtained directly by inserting Eq. (42) into Eq. (53). The end result is

$$\begin{aligned}
-\mathcal{L}_Y = & \frac{1}{v} \bar{D} \left\{ M_D (q_{k1} P_R + q_{k1}^* P_L) + \frac{v}{\sqrt{2}} [q_{k2} \rho^{D\dagger} P_R + q_{k2}^* \rho^D P_L] \right\} D h_k \\
& + \frac{1}{v} \bar{U} \left\{ M_U (q_{k1} P_L + q_{k1}^* P_R) + \frac{v}{\sqrt{2}} [q_{k2}^* \rho^U P_R + q_{k2} \rho^{U\dagger} P_L] \right\} U h_k \\
& + \left\{ \bar{U} [K \rho^{D\dagger} P_R - \rho^{U\dagger} K P_L] D H^+ + \frac{\sqrt{2}}{v} \bar{U} [K M_D P_R - M_U K P_L] D G^+ + \text{H.c.} \right\}, \quad (58)
\end{aligned}$$

where there is an implicit sum over $k = 0, 1, 2, 3$ (and $h_0 \equiv G^0$).

As expected, the Higgs-quark Yukawa couplings depend only on invariant quantities, namely, M_Q and ρ^Q (for $Q = U, D$) and the invariant angles θ_{12}, θ_{13} , while all dependence on θ_{23} has canceled. Since ρ^Q is in general a complex matrix, Eq. (58) exhibits CP-violating neutral-Higgs-fermion interactions. Moreover, Higgs-mediated FCNCs are present at tree level in cases where the ρ^Q are not flavor diagonal.

To avoid tree-level Higgs-mediated FCNCs, we shall impose a \mathbb{Z}_2 symmetry on the Higgs Lagrangian specified by Eqs. (2), (5), and (53). If the scalar potential respects the discrete symmetry $\Phi_1 \rightarrow \Phi_1$ and $\Phi_2 \rightarrow -\Phi_2$, then it follows that $m_{12}^2 = \lambda_6 = \lambda_7 = 0$. However, phenomenological considerations allow for the presence of a soft \mathbb{Z}_2 -breaking term, $m_{12}^2 \neq 0$. Consequently, we shall henceforth apply the \mathbb{Z}_2 symmetry exclusively to the dimension-four terms of the Higgs Lagrangian. Note that the action of the \mathbb{Z}_2 symmetry on the scalar fields is basis dependent. In Sec. V, we shall recast this action in a basis-independent form.

One must also impose the \mathbb{Z}_2 symmetry on the Yukawa Lagrangian, which defines the so-called \mathbb{Z}_2 basis. Four possible \mathbb{Z}_2 charge assignments are exhibited in Table II,

$$\text{Type Ia: } h_1^U = h_1^D = 0, \quad \text{Type Ib: } h_2^U = h_2^D = 0, \quad (59)$$

$$\text{Type IIa: } h_1^U = h_2^D = 0, \quad \text{Type IIb: } h_2^U = h_1^D = 0. \quad (60)$$

Of course, the above conditions are basis dependent. Types Ia and Ib (collectively denoted by Type I) and Types IIa and IIb (collectively denoted by Type II) are essentially equivalent, respectively, differing only in which scalar is denoted by Φ_1 and which is denoted by Φ_2 . In Ref. [34], the following basis-independent conditions were given:

$$\text{Type I: } \epsilon_{\bar{a}b} h_a^D h_b^U = \epsilon_{ab} h_{\bar{a}}^{D\dagger} h_b^{U\dagger} = 0, \quad (61)$$

$$\text{Type II: } \delta_{\bar{a}b} h_{\bar{a}}^{D\dagger} h_b^U = 0, \quad (62)$$

which are clearly satisfied in the \mathbb{Z}_2 basis. Employing Eq. (55) yields the invariant conditions,

$$\text{Type I: } \kappa^D \rho^U - \kappa^U \rho^D = 0, \quad (63)$$

$$\text{Type II: } \kappa^D \kappa^U + \rho^{D\dagger} \rho^U = 0, \quad (64)$$

where we have used the fact that κ^Q is a real matrix [cf. Eq. (57)].

In the \mathbb{Z}_2 basis, Eq. (3) yields $\hat{v} = (\cos \beta, e^{i\xi} \sin \beta)$ and $\hat{w} = (-e^{-i\xi} \sin \beta, \cos \beta)$, where $\tan \beta \equiv |v_2|/|v_1|$. Hence, using Eqs. (54) and (57), one obtains

TABLE II. Four possible \mathbb{Z}_2 charge assignments that forbid tree-level Higgs-mediated FCNC effects in the 2HDM Higgs-quark Yukawa interactions and the corresponding invariant Yukawa coupling matrix parameters. The Type Ia and Ib cases (collectively referred to as Type I) and the Type IIa and IIb cases (collectively referred to as Type II) differ, respectively, by the interchange of $\Phi_1 \rightarrow \Phi_2$ or equivalently by the interchange of $\cot \beta \rightarrow \tan \beta$. The presence of the \mathbb{Z}_2 symmetry fixes ρ^U and ρ^D to be diagonal matrices as exhibited below.

	Φ_1	Φ_2	U_R	D_R	U_L, D_L	ρ^U	ρ^D
Type Ia	+	-	-	-	+	$e^{i(\xi+\theta_{23})}(\sqrt{2}M_U/v) \cot \beta$	$e^{i(\xi+\theta_{23})}(\sqrt{2}M_D/v) \cot \beta$
Type Ib	+	-	+	+	+	$-e^{i(\xi+\theta_{23})}(\sqrt{2}M_U/v) \tan \beta$	$-e^{i(\xi+\theta_{23})}(\sqrt{2}M_D/v) \tan \beta$
Type IIa	+	-	-	+	+	$e^{i(\xi+\theta_{23})}(\sqrt{2}M_U/v) \cot \beta$	$-e^{i(\xi+\theta_{23})}(\sqrt{2}M_D/v) \tan \beta$
Type IIb	+	-	+	-	+	$-e^{i(\xi+\theta_{23})}(\sqrt{2}M_U/v) \tan \beta$	$e^{i(\xi+\theta_{23})}(\sqrt{2}M_D/v) \cot \beta$

$$\text{Type Ia: } \rho^U = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U \cot \beta}{v}, \quad \rho^D = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D \cot \beta}{v}, \quad (65)$$

$$\text{Type Ib: } \rho^U = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U \tan \beta}{v}, \quad \rho^D = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D \tan \beta}{v}, \quad (66)$$

$$\text{Type IIa: } \rho^U = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U \cot \beta}{v}, \quad \rho^D = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D \tan \beta}{v}, \quad (67)$$

$$\text{Type IIb: } \rho^U = -\frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_U \tan \beta}{v}, \quad \rho^D = \frac{e^{i(\xi+\theta_{23})}\sqrt{2}M_D \cot \beta}{v}, \quad (68)$$

which we have also recorded in Table II. Indeed, ρ^U and ρ^D are proportional to the diagonal quark matrices M_U and M_D , respectively, indicating that the tree-level Higgs-quark couplings are flavor diagonal. Since the ρ^Q are basis invariants, the quantity, $e^{i(\xi+\theta_{23})} \tan \beta$, is a physical parameter in the 2HDM with Type-I or Type-II Yukawa couplings.

In particular, note that one still has the freedom to make a transformation that interchanges $\Phi_1 \leftrightarrow \Phi_2$ in the \mathbb{Z}_2 basis. In performing such a basis transformation, one must also interchange $\tan \beta \leftrightarrow \cot \beta$ while changing the sign of the quantity $e^{i(\xi+\theta_{23})}$ [as we shall demonstrate in Eq. (75)]. These two parameter transformations simply result in the interchange of the a and b versions of the Type-I and Type-II Yukawa couplings. Once a specific discrete symmetry is chosen (among the four specified in Table II), $\tan \beta$ is promoted to a physical parameter of the model. It then follows that $e^{i(\xi+\theta_{23})}$ is also physical. However, the parameters ξ and θ_{23} separately retain their basis-dependent nature.

In contrast, the parameter $\tan \beta$ does not appear in the bosonic couplings of the 2HDM. This statement is easily checked by inserting Eq. (42) into Eqs. (2) and (5), which yields the Higgs self-couplings and the Higgs couplings to vector bosons [34]. The couplings of the Higgs bosons to the gauge bosons depend only on the gauge couplings and the invariant mixing angles θ_{12} and θ_{13} by virtue of Eqs. (5) and (42).⁷ The Higgs self-couplings will additionally depend on invariant combinations of the Z_i and $e^{-i\theta_{23}}$. If there exists a scalar field basis in which $\lambda_6 = \lambda_7 = 0$, then this basis is related to the Higgs basis by a rotation by the angle β . The existence of such a basis will yield an invariant relation among the Z_i that will be derived in the next section. It is only through this relation [cf. Eqs. (82) and

(83)] that $\tan \beta$ can be indirectly probed via the Higgs self-couplings.

V. BASIS-INDEPENDENT TREATMENT OF THE \mathbb{Z}_2 SYMMETRY

The \mathbb{Z}_2 symmetry of the 2HDM scalar potential is manifestly realized in a scalar field basis where $m_{12}^2 = \lambda_6 = \lambda_7 = 0$, and is softly broken if $m_{12}^2 \neq 0$ in a basis where $\lambda_6 = \lambda_7 = 0$. Of course, such a description is basis dependent. In this section, we explore a basis-independent characterization of the \mathbb{Z}_2 symmetry, where the symmetry is either exact or softly broken. We obtain conditions in terms of Higgs basis parameters that are independent of the initial choice of scalar field basis. Our analysis generalizes results previously obtained in Refs. [25,45,46]. The connection of the results obtained in this section with the basis-independent conditions that are independent of the vacuum, derived in Ref. [33], is discussed in Appendix C. An alternative basis-independent treatment of the \mathbb{Z}_2 symmetry based on the bilinear formalism of the 2HDM scalar potential can be found in Refs. [36,39,40].

A. The inert doublet model

A very special case of the 2HDM is the so-called inert doublet model (IDM). In this model, the Higgs basis exhibits an exact \mathbb{Z}_2 symmetry, $\mathcal{H}_1 \rightarrow \mathcal{H}_1$ and $\mathcal{H}_2 \rightarrow -\mathcal{H}_2$. Imposing this symmetry on the scalar potential given in Eq. (28) yields

$$Y_3 = Z_6 = Z_7 = 0. \quad (69)$$

The conditions given in Eq. (69) are basis independent given that Y_3 , Z_6 , and Z_7 are pseudo-invariant quantities. Note that it is sufficient to impose the \mathbb{Z}_2 symmetry on the dimension-four terms of Eq. (28), since if $Z_6 = 0$ then $Y_3 = 0$ due to the scalar potential minimum conditions of Eq. (24). Thus, in this case, it is not possible to softly break the \mathbb{Z}_2 symmetry.

To complete the definition of the IDM, the Higgs-fermion Yukawa couplings are fixed by imposing the

⁷Note that the Type-I or Type-II conditions remove two of the four gauge invariant Yukawa couplings [cf. Eqs. (59) and (60)], which ultimately provide meaning for the parameter $\tan \beta$. In contrast, the imposition of the (softly broken) \mathbb{Z}_2 symmetry does *not* remove any of the Higgs boson–gauge boson couplings, whose forms are fixed by gauge invariance.

condition that all fermion fields are even under the \mathbb{Z}_2 symmetry. This corresponds to Type-Ib Yukawa couplings as specified in Table II with $\tan\beta = 0$. In this case, $\rho^U = \rho^D = 0$, which implies that the doublet \mathcal{H}_2 does not couple to the fermions. Consequently, \mathcal{H}_2 is called an inert doublet. Due to the fact that $Z_6 = 0$, the tree-level couplings of the neutral scalar that resides in the doublet \mathcal{H}_1 are precisely those of the SM Higgs boson. Moreover, in the bosonic sector of the theory, the scalar fields that reside in the doublet \mathcal{H}_2 can only couple in pairs to the gauge bosons and to the SM Higgs boson.

In light of Eq. (69), Z_5 is the only potentially complex parameter of the IDM scalar potential. This means that one is free to rephase the pseudoinvariant Higgs basis field H_2 such that all Higgs basis scalar potential parameters are real. Hence, the IDM scalar potential and vacuum are CP conserving. Since the main interest of this paper is the 2HDM with a softly broken \mathbb{Z}_2 symmetry and CP violation, we shall henceforth assume that the \mathbb{Z}_2 symmetry of the dimension-four terms of the scalar potential is manifestly realized in a basis that is not the Higgs basis. That is, Z_6 and Z_7 are not both simultaneously equal to zero. This assumption will allow for the possibility of a 2HDM scalar sector that exhibits either explicit or spontaneous CP violation.

B. A softly broken \mathbb{Z}_2 symmetry

Suppose that the \mathbb{Z}_2 symmetry of the dimension-four terms of the scalar potential is manifestly realized in some scalar field basis (henceforth denoted as the \mathbb{Z}_2 basis), which implies that $\lambda_6 = \lambda_7 = 0$ in this basis. In light of Eqs. (A29) and (A30), it follows that the \mathbb{Z}_2 basis exists if and only if values of β and ξ can be found such that

$$\frac{1}{2}s_{2\beta}(Z_1 - Z_2) + c_{2\beta}\text{Re}(Z_{67}e^{i\xi}) + i\text{Im}(Z_{67}e^{i\xi}) = 0, \quad (70)$$

$$\begin{aligned} & \frac{1}{2}s_{2\beta}c_{2\beta}[Z_1 + Z_2 - 2Z_{34} - 2\text{Re}(Z_5e^{2i\xi})] \\ & - is_{2\beta}\text{Im}(Z_5e^{2i\xi}) + c_{4\beta}\text{Re}[(Z_6 - Z_7)e^{i\xi}] \\ & + ic_{2\beta}\text{Im}[(Z_6 - Z_7)e^{i\xi}] = 0, \end{aligned} \quad (71)$$

where $Z_{34} \equiv Z_3 + Z_4$ and $Z_{67} \equiv Z_6 + Z_7$. The real and imaginary parts of Eqs. (70) and (71) yield four independent real equations.

The \mathbb{Z}_2 basis is not unique. Suppose, we choose a Φ basis in which $\lambda_6 = \lambda_7 = 0$. To maintain the conditions, $\lambda_6 = \lambda_7 = 0$, it is still possible to transform to a new Φ' basis that is related to the Φ basis according to $\Phi'_a = U_{ab}\Phi_b$, where

$$U = \begin{pmatrix} 0 & e^{-i\xi} \\ e^{i\xi} & 0 \end{pmatrix}. \quad (72)$$

In particular, by noting that

$$\begin{pmatrix} s_\beta \\ c_\beta e^{i\xi} \end{pmatrix} = U \begin{pmatrix} c_\beta \\ s_\beta e^{i\xi} \end{pmatrix}, \quad (73)$$

it immediately follows that $\beta' = \frac{1}{2}\pi - \beta$ and $\xi' = \xi$. Moreover, after employing Eq. (20), where $\det U = -e^{i(\xi-\xi)}$, it follows that if $\Phi_a \rightarrow U_{ab}\Phi_b$ with U given by Eq. (72), then

$$\begin{aligned} Z_5 e^{2i\xi} &\rightarrow Z_5 e^{2i\xi}, & Z_6 e^{i\xi} &\rightarrow -Z_6 e^{i\xi}, \\ Z_7 e^{i\xi} &\rightarrow -Z_7 e^{i\xi}, & s_{2\beta} &\rightarrow s_{2\beta}, & c_{2\beta} &\rightarrow -c_{2\beta}. \end{aligned} \quad (74)$$

That is, the left-hand side of Eq. (70) [Eq. (71)] is transformed into [the negative of] its complex conjugate, and the four real equations obtained from Eqs. (70) and (71) are unchanged. Likewise, using Eq. (39), it follows that if $\Phi_a \rightarrow U_{ab}\Phi_b$ with U given by Eq. (72), then

$$e^{i(\xi+\theta_{23})} \rightarrow -e^{i(\xi+\theta_{23})}, \quad (75)$$

which shows that the phase factor, $e^{i(\xi+\theta_{23})}$, appearing in the expressions for ρ^Q exhibited in Eqs. (65)–(68), changes sign when transforming from the Φ basis to the Φ' basis. Consequently, the effect of this scalar field transformation is to interchange the a and b versions of the Type-I and Type-II Yukawa couplings as asserted below Eq. (68).

Returning to Eqs. (70) and (71), we first take the imaginary part of Eq. (70) to obtain

$$\text{Im}(Z_{67}e^{i\xi}) = 0. \quad (76)$$

Assuming that $Z_{67} \neq 0$ (we will return to the case of $Z_{67} = 0$ later), we shall denote

$$Z_{67} = |Z_{67}|e^{i\theta_{67}}. \quad (77)$$

Then, Eq. (76) implies that $\xi + \theta_{67} = n\pi$, for some integer n , or equivalently

$$e^{i\xi} = \pm e^{-i\theta_{67}}. \quad (78)$$

The two possible sign choices in Eq. (78) correspond to the Φ and Φ' basis choices identified above in which $\lambda_6 = \lambda_7 = 0$ is satisfied. Employing Eq. (78) in Eqs. (70) and (71) yields

$$\frac{1}{2}s_{2\beta}(Z_1 - Z_2) \pm c_{2\beta}|Z_{67}| = 0, \quad (79)$$

$$\begin{aligned} & \frac{1}{2}s_{2\beta}c_{2\beta}[Z_1 + Z_2 - 2Z_{34} - 2\text{Re}(Z_5e^{-2i\theta_{67}})] \\ & - is_{2\beta}\text{Im}(Z_5e^{-2i\theta_{67}}) \pm c_{4\beta}\text{Re}[(Z_6 - Z_7)e^{-i\theta_{67}}] \\ & \pm ic_{2\beta}\text{Im}[(Z_6 - Z_7)e^{-i\theta_{67}}] = 0. \end{aligned} \quad (80)$$

Assuming $Z_1 \neq Z_2$ (we will return to the case of $Z_1 = Z_2$ below), Eq. (79) yields

$$\frac{s_{2\beta}}{c_{2\beta}} = \pm \frac{2|Z_{67}|}{Z_2 - Z_1}. \quad (81)$$

$$\tan \beta = \sqrt{\frac{1 - c_{2\beta}}{1 + c_{2\beta}}}, \quad (83)$$

Since $0 \leq \beta \leq \frac{1}{2}\pi$, it follows that

$$\begin{aligned} s_{2\beta} &= \frac{2|Z_{67}|}{\sqrt{(Z_2 - Z_1)^2 + 4|Z_{67}|^2}}, \\ c_{2\beta} &= \frac{\pm(Z_2 - Z_1)}{\sqrt{(Z_2 - Z_1)^2 + 4|Z_{67}|^2}}. \end{aligned} \quad (82)$$

In particular,

which demonstrates that $\tan \beta$ in the Φ basis corresponds to $\cot \beta$ in the Φ' basis. Moreover,

$$e^{i(\xi + \theta_{23})} = \pm e^{i(\theta_{23} - \theta_{67})} = \pm \frac{|Z_{67}|}{Z_{67} e^{-i\theta_{23}}} = \left(\frac{Z_2 - Z_1}{2Z_{67} e^{-i\theta_{23}}} \right) \frac{s_{2\beta}}{c_{2\beta}}. \quad (84)$$

Note that Eq. (84) is consistent with the result of Eq. (75). Plugging the results of Eq. (82) back into Eq. (80),

$$\begin{aligned} &|Z_{67}|(Z_2 - Z_1)[Z_1 + Z_2 - 2Z_{34} - 2\text{Re}(Z_5 e^{-2i\theta_{67}})] + [(Z_2 - Z_1)^2 - 4|Z_{67}|^2]\text{Re}[(Z_6 - Z_7)e^{-i\theta_{67}}] \\ &\pm iD\{(Z_2 - Z_1)\text{Im}[(Z_6 - Z_7)e^{-i\theta_{67}}] - 2|Z_{67}|\text{Im}(Z_5 e^{-2i\theta_{67}})\} = 0, \end{aligned} \quad (85)$$

where $D \equiv \sqrt{(Z_2 - Z_1)^2 + 4|Z_{67}|^2}$. We can use Eq. (77) to write $e^{-i\theta_{67}} = Z_{67}^*/|Z_{67}|$. It then follows that

$$\begin{aligned} &(Z_2 - Z_1)[|Z_{67}|^2(Z_1 + Z_2 - 2Z_{34}) - 2\text{Re}(Z_5^* Z_{67}^2)] + [(Z_2 - Z_1)^2 - 4|Z_{67}|^2][|Z_6|^2 - |Z_7|^2] \\ &\pm 2iD\{(Z_1 - Z_2)\text{Im}(Z_6^* Z_7) + \text{Im}(Z_5^* Z_{67}^2)\} = 0. \end{aligned} \quad (86)$$

Taking the real and imaginary parts of Eq. (86) and massaging the real part yield

$$(Z_1 - Z_2)[Z_{34}|Z_{67}|^2 - Z_2|Z_6|^2 - Z_1|Z_7|^2 - (Z_1 + Z_2)\text{Re}(Z_6^* Z_7) + \text{Re}(Z_5^* Z_{67}^2)] - 2|Z_{67}|^2(|Z_6|^2 - |Z_7|^2) = 0, \quad (87)$$

$$(Z_1 - Z_2)\text{Im}(Z_6^* Z_7) + \text{Im}(Z_5^* Z_{67}^2) = 0. \quad (88)$$

It is convenient to multiply Eq. (88) by $-i$ and add the result to Eq. (87). This yields a single complex equation. Finally, since $Z_{67} \neq 0$ by assumption, one can divide this complex equation by Z_{67}^* and take the complex conjugate of the result to obtain

$$(Z_1 - Z_2)[Z_{34}Z_{67}^* - Z_1Z_7^* - Z_2Z_6^* + Z_5^*Z_{67}] - 2Z_{67}^*(|Z_6|^2 - |Z_7|^2) = 0. \quad (89)$$

The cases where $Z_1 = Z_2$ and/or $Z_{67} = 0$ are easily treated. First, if $Z_1 = Z_2$ and $Z_{67} \neq 0$, then Eqs. (79) and (80) imply that $s_{2\beta} = 1$ and $c_{2\beta} = 0$, and it follows that $\text{Im}(Z_5^* Z_{67}^2) = 0$ and $|Z_6| = |Z_7|$. Second, if $Z_{67} = 0$ and $Z_1 \neq Z_2$, then Eq. (70) yields $s_{2\beta} = 0$, which when inserted into Eq. (71) implies that $Z_6 e^{i\xi} = 0$. That is, if $Z_{67} = 0$, then $Z_6 = Z_7 = 0$, and the Z_2 symmetry is manifest in the Higgs basis, as noted in Sec. VA. In this latter case, one must employ the Type-Ib Yukawa interactions, which yield $\rho^U = \rho^D = 0$. This corresponds to the case of $\tan \beta = 0$ in Eq. (66).⁸ Likewise, in the case of Type-II couplings, $M_U = \rho^D = 0$ and ρ^U is an arbitrary complex matrix. In the IDM (corresponding to a Type-Ib Yukawa sector with

$Z_6 = Z_7 = 0$), the fermions couple only to the Z_2 -even scalar doublet \mathcal{H}_1 , whose tree-level interactions exactly coincide with those of the SM Higgs doublet.

Finally, the case of $Z_1 = Z_2$ and $Z_{67} = 0$ requires special treatment; this case has been dubbed the ‘‘exceptional region’’ of the 2HDM parameter space in Ref. [47]. The analysis of Appendix B shows that in this exceptional case, there always exists a scalar field basis in which the softly broken Z_2 symmetry is manifestly realized. Furthermore, Eqs. (88) and (89) are trivially satisfied in the exceptional region of the 2HDM parameter space.

In conclusion, Eq. (89) is a necessary condition for the presence of a softly broken Z_2 symmetry. It is also a sufficient condition in all cases with one exception. Namely, if $Z_1 = Z_2$, $Z_5 \neq 0$, and $Z_{67} \neq 0$, then Eq. (89) must be supplemented with the additional constraint of $\text{Im}(Z_5^* Z_{67}^2) = 0$.

⁸If one were to employ Type-Ia Yukawa couplings, then one would find that $M_U = M_D = 0$, while ρ^U and ρ^D are arbitrary complex matrices.

In the case of the CP-conserving 2HDM, it is possible to rephase the pseudoinvariant Higgs basis field H_2 such that all of the Z_i are real. In this real basis, Eq. (89) reduces to

$$(Z_1 - Z_2)[(Z_{34} + Z_5)Z_{67} - Z_2Z_6 - Z_1Z_7] - 2Z_{67}^2(Z_6 - Z_7) = 0, \quad (90)$$

a result previously given in eq. (54) of Ref. [45]. The scalar basis in which $\lambda_6 = \lambda_7 = 0$ is obtained from the Higgs basis by a rotation by an angle β , which is determined by Eq. (81),

$$\cot 2\beta = \frac{Z_2 - Z_1}{2Z_{67}}, \quad (91)$$

in a convention where v_1 and v_2 are non-negative [in which case $\xi = 0$ so that $\text{sgn}Z_{67} = \pm 1$ in light of Eq. (78)]. Once again, the exceptional region of parameter space where $Z_1 = Z_2$ and $Z_{67} = 0$ must be treated separately. Using Eqs. (B2) and (B3) with $\xi = 0$ and real Z_i , it follows that $\cot 2\beta$ is a solution of Eq. (B7), where Z_5 and Z_6 are real and \pm is identified with $\text{sgn}Z_6$ (or equivalently, replace $|Z_6|$ with Z_6 and replace \pm with a plus sign).

C. Softly broken \mathbb{Z}_2 symmetry and spontaneously broken CP symmetry

Suppose that the conditions for a softly broken \mathbb{Z}_2 -symmetric scalar potential obtained in Sec. VB are satisfied. Then a \mathbb{Z}_2 basis exists (which is not unique) in which $\lambda_6 = \lambda_7 = 0$. If in addition,

$$\text{Im}(\lambda_5^*[m_{12}^2]^2) = 0, \quad (92)$$

then one can rephase one of the scalar fields such that m_{12}^2 and λ_5 are simultaneously real. In this case, the scalar potential is explicitly CP invariant. In addition, if in this so-called real \mathbb{Z}_2 basis there is an unremovable complex phase in the vevs, that is,

$$\text{Im}(v_1^*v_2) = \frac{1}{2}v^2s_{2\beta}\sin\xi \neq 0, \quad (93)$$

then the CP symmetry of the scalar potential is spontaneously broken.

Using Eqs. (A20) and (A25),

$$\begin{aligned} \text{Im}(\lambda_5^*[m_{12}^2]^2) &= \left\{ \frac{1}{4}s_{2\beta}^2[Z_1 + Z_2 - 2Z_{345}] + \text{Re}(Z_5e^{2i\xi}) + s_{2\beta}c_{2\beta}\text{Re}[(Z_6 - Z_7)e^{i\xi}] \right\} \\ &\quad \times [(Y_1 - Y_2)s_{2\beta} + 2\text{Re}(Y_3e^{i\xi})c_{2\beta}]\text{Im}(Y_3e^{i\xi}) \\ &\quad - \left\{ \frac{1}{4}[(Y_1 - Y_2)s_{2\beta} + 2\text{Re}(Y_3e^{i\xi})c_{2\beta}]^2 - [\text{Im}(Y_3e^{i\xi})]^2 \right\} \\ &\quad \times [c_{2\beta}\text{Im}(Z_5e^{2i\xi}) + s_{2\beta}\text{Im}[(Z_6 - Z_7)e^{i\xi}]], \end{aligned} \quad (94)$$

where $Z_{345} \equiv Z_{34} + \text{Re}(Z_5e^{2i\xi})$. Next, we employ the potential minimum conditions [Eq. (24)], $Y_1 = -\frac{1}{2}Z_1v^2$ and $Y_3 = -\frac{1}{2}Z_6v^2$, and we make use of Eq. (82) for $s_{2\beta}$ and $c_{2\beta}$. To make further progress, we first assume that $Z_1 \neq Z_2$ and $Z_{67} \neq 0$. In this case, we can use Eqs. (77) and (78) to write $e^{i\xi} = \pm Z_{67}^*/|Z_{67}|$. It is convenient to introduce the following notation:

$$f_1 \equiv |Z_{67}|^2, \quad f_2 \equiv |Z_7|^2 - |Z_6|^2, \quad f_3 \equiv \text{Im}(Z_6Z_7^*). \quad (95)$$

It then follows that

$$\text{Re}(Z_6e^{i\xi}) = \pm \frac{\text{Re}(Z_6Z_7^*) + |Z_6|^2}{|Z_{67}|} = \pm \frac{1}{2}(f_1 - f_2)f_1^{-1/2}, \quad (96)$$

$$\text{Im}(Z_6e^{i\xi}) = \pm \frac{\text{Im}(Z_6Z_7^*)}{|Z_{67}|} = \pm f_3f_1^{-1/2}, \quad (97)$$

$$\text{Re}[(Z_6 - Z_7)e^{i\xi}] = \pm \left(\frac{|Z_6|^2 - |Z_7|^2}{|Z_{67}|} \right) = \mp f_2f_1^{-1/2}, \quad (98)$$

$$\text{Im}[(Z_6 - Z_7)e^{i\xi}] = \pm \frac{2\text{Im}(Z_6Z_7^*)}{|Z_{67}|} = \pm 2f_3f_1^{-1/2}. \quad (99)$$

Finally, we employ Eqs. (87) and (88) to obtain

$$\begin{aligned} \text{Re}(Z_5e^{2i\xi}) &= \frac{\text{Re}(Z_5^*Z_{67}^2)}{|Z_{67}|^2} = \frac{2f_2}{Z_2 - Z_1} + \frac{1}{2}(Z_1 + Z_2) \\ &\quad - Z_{34} + \frac{(Z_1 - Z_2)f_2}{2f_1}, \end{aligned} \quad (100)$$

$$\text{Im}(Z_5e^{2i\xi}) = -\frac{\text{Im}(Z_5^*Z_{67}^2)}{|Z_{67}|^2} = \frac{(Z_2 - Z_1)f_3}{f_1}. \quad (101)$$

Plugging the above results into Eq. (94), we end up with

$$\text{Im}(\lambda_5^*[m_{12}^2]^2) = \mp \frac{v^4 f_3 \mathcal{F}}{16f_1^2(Z_1 - Z_2)\sqrt{(Z_2 - Z_1)^2 + 4f_1}}, \quad (102)$$

where the function \mathcal{F} is given by⁹

$$\begin{aligned} \mathcal{F} = f_1^2 & \left[16(Z_1 - Z_2) \left(\frac{Y_2}{v^2} \right)^2 + 16[f_2 + (Z_1 - Z_2)Z_{34}] \left(\frac{Y_2}{v^2} \right) + 4f_2(Z_1 + Z_2) - (Z_1^2 - Z_2^2)(Z_1 + Z_2 - 4Z_{34}) \right] \\ & - (f_2^2 + 4f_3^2)(Z_1 - Z_2)^3 - 2f_1 f_2 (Z_1 - Z_2)^2 (Z_1 + Z_2 - 2Z_{34}) + 4f_1 (f_2^2 - 4f_3^2)(Z_1 - Z_2). \end{aligned} \quad (103)$$

Thus, $\text{Im}(\lambda_5^*[m_{12}^2]^2) = 0$ if one of two conditions are satisfied: $f_3 = 0$ and/or $\mathcal{F} = 0$. If $f_3 = 0$, then it follows that $\text{Im}(Z_5 e^{2i\xi}) = \text{Im}(Z_6 e^{i\xi}) = \text{Im}(Z_7 e^{i\xi}) = 0$. This implies that one can rephase the Higgs basis field H_2 such that Z_5 , Z_6 , and Z_7 are simultaneously real [which also implies that Y_3 is real by Eq. (24)]. That is, all the coefficients of the scalar potential in the Higgs basis and the corresponding vevs are real, implying that the scalar potential and the vacuum are CP conserving. In contrast, if $f_3 \neq 0$ and $\mathcal{F} = 0$, then the scalar potential is explicitly CP conserving as noted below Eq. (92). However, in the \mathbb{Z}_2 basis in which all scalar potential parameters are real, the vevs exhibit a complex phase that cannot be removed by a basis transformation while maintaining real coefficients in the scalar potential. In particular, $\text{Im}(Z_6 Z_7^*) \neq 0$ implies that no real Higgs basis exists, which is a signal of CP violation.¹⁰ Thus, $f_3 \neq 0$ and $\mathcal{F} = 0$ is a basis-independent signal of spontaneous CP violation.¹¹

If $\mathcal{F} = 0$, then Eq. (103) provides a quadratic equation for Y_2 that yields $Y_2 \sim \mathcal{O}(Z_i)$. In contrast, the decoupling limit of the 2HDM corresponds to $Y_2 \gg v$ [34]. Since $|Z_i|/4\pi \lesssim \mathcal{O}(1)$ as a consequence of tree-level unitarity [49–55], it follows that the 2HDM with a softly broken \mathbb{Z}_2 symmetry and spontaneous CP violation possesses no decoupling limit [56].

⁹An expression for \mathcal{F} was first derived by Lavoura in Ref. [46], although his eq. (22) contains a misprint in which the factor of f_2 in the coefficient of $(Z_1 - Z_2)^2(Z_1 + Z_2 - 2Z_{34})$ in Eq. (103) was inadvertently dropped.

¹⁰We define a real Higgs basis to be the basis in which the potentially complex parameters Z_5 , Z_6 , and Z_7 are simultaneously real. In this case, Y_3 is also real in light of Eq. (24). Note that a real Higgs basis exists if and only if $\text{Im}(Z_6^2 Z_5^*) = \text{Im}(Z_7^2 Z_5^*) = \text{Im}(Z_6 Z_7^*) = 0$, in which case one can rephase the Higgs basis field H_2 appropriately to achieve the real Higgs basis. In the 2HDM, the existence of a real Higgs basis is a necessary and sufficient condition for a CP-conserving scalar potential and vacuum.

¹¹Basis-independent conditions for spontaneous CP violation have also been obtained in the bilinear formalism of the 2HDM in Refs. [37,38].

To complete the analysis of this subsection, we must address the special cases in which either $Z_1 = Z_2$ and/or $Z_{67} = 0$. As noted below Eq. (89), if $Z_1 = Z_2$ and $Z_{67} \neq 0$, then Eqs. (79) and (80) imply that $s_{2\beta} = 1$ and $c_{2\beta} = 0$, and it follows that $\text{Im}(Z_5^* Z_{67}^2) = 0$ and $|Z_6| = |Z_7|$ in light of Eqs. (87) and (88). Then, Eq. (94) yields

$$\begin{aligned} \text{Im}(\lambda_5^*[m_{12}^2]^2) & = \mp \frac{v^4 f_3}{8f_1^{3/2}} \left\{ f_1 \left[4 \left(\frac{Y_2}{v^2} \right)^2 + \frac{2Y_2}{v^2} (Z_1 + Z_{34}) + Z_1 Z_{34} \right] \right. \\ & \quad \left. - 4f_3^2 - \left(Z_1 + \frac{2Y_2}{v^2} \right) \text{Re}(Z_5^* Z_{67}^2) \right\}. \end{aligned} \quad (104)$$

Note that in contrast to Eq. (100), $\text{Re}(Z_5^* Z_{67}^2)$ is not determined in terms of the Z_i , f_1 , and f_2 , since in the case of $Z_1 = Z_2$, this quantity is not constrained by Eqs. (87) and (88). Indeed, another way to derive Eq. (104) is to use Eq. (100) to solve for f_2 in terms of $\text{Re}(Z_5^* Z_{67}^2)$ and substitute this result back into Eq. (103). In this way, the factor of $Z_1 - Z_2$ in the denominator of Eq. (102) is canceled. The resulting expression is significantly more complicated than the one given in Eq. (103). Nevertheless, by setting $Z_1 = Z_2$ in this latter expression, we have checked that one recovers the result of Eq. (104). Thus, we again conclude that spontaneous CP violation occurs if $f_3 \neq 0$ and the following basis-independent condition is satisfied:

$$\begin{aligned} f_1 & \left[4 \left(\frac{Y_2}{v^2} \right)^2 + \frac{2Y_2}{v^2} (Z_1 + Z_{34}) + Z_1 Z_{34} \right] \\ & - 4f_3^2 - \left(Z_1 + \frac{2Y_2}{v^2} \right) \text{Re}(Z_5^* Z_{67}^2) = 0. \end{aligned} \quad (105)$$

Next, as noted below Eq. (89), if $Z_{67} = 0$ and $Z_1 \neq Z_2$, then Eqs. (70) and (71) imply that $Z_6 = Z_7 = 0$. Thus, an unbroken \mathbb{Z}_2 symmetry is manifestly realized in the Higgs basis. That is, in this case, one identifies $m_{12}^2 = 0$ and thus $\text{Im}(\lambda_5^*[m_{12}^2]^2) = 0$ is trivially satisfied. Moreover, one can rephase the Higgs basis field H_2 such that Z_5 is real. Hence,

a real Higgs basis exists which implies that both the scalar potential and the vacuum are CP conserving.

So far, in all cases considered above, the conditions $\lambda_6 = \lambda_7 = 0$ and $\text{Im}(\lambda_5^*[m_{12}^2]^2) = 0$ in the Φ basis were necessary and sufficient for an explicitly CP-conserving scalar potential. One encounters a surprising result when considering the final case of the exceptional region of parameter space, where $Z_1 = Z_2$ and $Z_7 = -Z_6 \neq 0$, where the only potentially CP-violating invariant is $\text{Im}(Z_5^*Z_6^2)$. Suppose that the Higgs basis parameters satisfy $\text{Im}(Z_5^*Z_6^2) = 0$, $Z_1 = Z_2$ and $Z_7 = -Z_6 \neq 0$. Then, there exists a Φ basis that satisfies $\lambda_6 = \lambda_7 = 0$, $\beta = \frac{1}{4}\pi$, and $\cos(\xi + \theta_6) = 0$, where $\theta_6 = \arg Z_6$. It follows that

$$\begin{aligned} \text{Im}(Z_5 e^{2i\xi}) &= \frac{\text{Im}(Z_5^*Z_6^2)}{|Z_6|^2} = 0, \\ \text{Re}(Z_6 e^{i\xi}) &= \text{Re}(Z_7 e^{i\xi}) = 0, \\ \text{Re}(Z_5 e^{2i\xi}) &= -\frac{\text{Re}(Z_5^*Z_6^2)}{|Z_6|^2}, \\ \text{Im}(Z_6 e^{i\xi}) &= -\text{Im}(Z_7 e^{i\xi}) = \pm|Z_6|, \end{aligned} \quad (106)$$

$$\text{Im}(Z_5 e^{2i\xi}) = -\frac{\text{Re}(Z_5^*Z_6^2)}{|Z_6|^2}, \quad (107)$$

where the sign choice in Eq. (107) is correlated with $\sin(\xi + \theta_6) = \pm 1$. In light of Eqs. (A26) and (A27), it follows that $\lambda_6 = \lambda_7 = 0$. If we now insert the above results into Eqs. (A20) and (A25) and employ the scalar potential minimum conditions [Eq. (24)], then

$$\begin{aligned} m_{12}^2 e^{i\xi} &= \frac{1}{4} v^2 \left[\left(Z_1 + \frac{2Y_2}{v^2} \right) \pm 2i|Z_6| \right], \\ \lambda_5 e^{2i\xi} &= \frac{1}{2} \left[Z_1 - Z_{34} - \frac{\text{Re}(Z_5^*Z_6^2)}{|Z_6|^2} \right] \pm 2i|Z_6|. \end{aligned} \quad (108)$$

Hence, for generic choices of the remaining scalar potential parameters, one can conclude that a parameter regime within the exceptional region of the parameter space exists where

$$\begin{aligned} \text{Im}(\lambda_5^*[m_{12}^2]^2) &= \pm \frac{v^4}{8|Z_6|} \left\{ |Z_6|^2 \left[4|Z_6|^2 - \left(Z_1 + \frac{2Y_2}{v^2} \right)^2 \right] \right. \\ &\quad \left. + \left(Z_1 + \frac{2Y_2}{v^2} \right) [|Z_6|^2(Z_1 - Z_{34}) - \text{Re}(Z_5^*Z_6^2)] \right\} \neq 0, \end{aligned} \quad (109)$$

in which the scalar potential is explicitly CP conserving, and moreover CP is not spontaneously broken! In this case, CP is conserved despite the fact that no \mathbb{Z}_2 basis exists in which all the scalar potential parameters are real (for further details, see Ref. [57]).

In the exceptional region of parameter space where $\lambda_6 = \lambda_7 = 0$ is achieved for $\beta \neq \frac{1}{4}\pi$, one finds once again that $\text{Im}(\lambda_5^*[m_{12}^2]^2) = 0$ is both a necessary and sufficient condition for an explicit CP-conserving scalar potential. Moreover, if $\text{Im}(\lambda_5^*[m_{12}^2]^2) = 0$ and $\text{Im}(Z_5^*Z_6^2) \neq 0$, then CP is spontaneously broken. Further details are provided at the end of Appendix B.

D. Imposing the convention of non-negative real vevs in the Z_2 basis

In some applications, it is convenient to adopt a convention in which $\xi = 0$ in the basis where $\lambda_6 = \lambda_7 = 0$. If this condition is not satisfied initially, it is straightforward to impose this condition by an appropriate rephasing of the Higgs-doublet field Φ_2 . In this convention, the real and imaginary parts of Eqs. (70) and (71) yield

$$\frac{1}{2} s_{2\beta} (Z_1 - Z_2) + c_{2\beta} \text{Re} Z_{67} = 0, \quad (110)$$

$$\text{Im} Z_{67} = 0, \quad (111)$$

$$\frac{1}{2} s_{2\beta} c_{2\beta} [Z_1 + Z_2 - 2Z_{34} - 2\text{Re} Z_5] + c_{4\beta} \text{Re}(Z_6 - Z_7) = 0, \quad (112)$$

$$s_{2\beta} \text{Im} Z_5 - c_{2\beta} \text{Im}(Z_6 - Z_7) = 0. \quad (113)$$

Equations (110)–(112) are equivalent to eq. (3.16) of Ref. [58]. Because we have fixed $\xi = 0$ in the Φ basis, we must choose $\xi = \zeta = 0$ in Eq. (72) in defining the Φ' basis in order to maintain our convention in which the vevs v_1 and v_2 are real and non-negative. That is, $\Phi'_a = U_{ab} \Phi_b$ where $U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Since $\det U = -1$, it follows that pseudoinvariant quantities will change sign between the Φ and Φ' bases. Indeed, the effect of transforming from the Φ basis to the Φ' basis is to modify the Φ -basis parameters such that

$$\begin{aligned} m_{11}^2 &\leftrightarrow m_{22}^2, & m_{12}^2 &\rightarrow m_{12}^{2*}, & \lambda_1 &\leftrightarrow \lambda_2, \\ \lambda_5 &\rightarrow \lambda_5^*, & v_1 &\leftrightarrow v_2, \end{aligned} \quad (114)$$

whereas λ_3 , λ_4 , and $\lambda_6 = \lambda_7 = 0$ are unchanged. In light of Eq. (20), the Higgs basis parameters obtained starting from the Φ' basis differ from those obtained starting from the Φ basis by the following sign changes:

$$\{Y_3, Z_6, Z_7\} \rightarrow \{-Y_3, -Z_6, -Z_7\}, \quad (115)$$

In particular, the Higgs basis parameter Z_5 is *unchanged* since $(\det U)^2 = 1$.

As previously noted, $\tan\beta$ is not yet a physical parameter, since the effect of transforming from the Φ basis to the Φ' basis is to modify $\beta \rightarrow \frac{1}{2}\pi - \beta$. In light of these remarks,

one can check that Eqs. (110)–(113) are invariant with respect to the transformation $\Phi'_a = U_{ab}\Phi_b$, and thus define the invariant conditions for the existence of a scalar field basis with $\lambda_6 = \lambda_7 = 0$ and non-negative real scalar vevs (i.e., $\xi = 0$).

Consider first the case of $Z_{67} \neq 0$. By virtue of Eq. (111), it follows that the pseudo-invariant quantity Z_{67} is real. This condition fixes the Higgs basis up to a twofold ambiguity that depends on the sign of Z_{67} . This ambiguity is simply a consequence of the freedom to change from the Φ basis to the Φ' basis, while maintaining the \mathbb{Z}_2 -basis conditions, $\lambda_6 = \lambda_7 = 0$, as discussed above. Likewise, the pseudoinvariant quantity $e^{i\theta_{23}}$ is determined up to a twofold ambiguity, as its sign can be flipped by transforming from the Φ basis to the Φ' basis.

One can obtain an explicit expression for $e^{i\theta_{23}}$ in terms of pseudoinvariant quantities by setting $\xi = 0$ in Eq. (84),

$$e^{i\theta_{23}} = \left(\frac{Z_2 - Z_1}{2Z_{67}e^{-i\theta_{23}}} \right) \frac{s_{2\beta}}{c_{2\beta}}. \quad (116)$$

Under $\Phi_1 \leftrightarrow \Phi_2$, $c_{2\beta}$ changes sign, and we conclude that θ_{23} is determined modulo π . However, a more practical expression can be obtained as follows. Writing $Z_6 \equiv |Z_6|e^{i\theta_6}$ and $Z_7 \equiv |Z_7|e^{i\theta_7}$, Eq. (111) is equivalent to the equation, $|Z_6|\sin\theta_6 + |Z_7|\sin\theta_7 = 0$. One can eliminate θ_7 and solve for θ_6 to obtain

$$\tan\theta_6 = \frac{\text{Im}(Z_6Z_7^*)}{|Z_6|^2 + \text{Re}(Z_6Z_7^*)}, \quad (117)$$

which implies that θ_6 is determined modulo π . Under the assumption that $Z_6 \neq 0$, one can obtain an explicit formula for $e^{i\theta_{23}}$,

$$e^{i\theta_{23}} = \frac{|Z_6|e^{i\theta_6}}{Z_6e^{-i\theta_{23}}}, \quad (118)$$

where the numerator and denominator on the right-hand side of Eq. (118) are evaluated by employing Eqs. (117) and (50), respectively. As expected, θ_{23} is thus determined modulo π .

If $Z_6 = 0$, then Eq. (111) yields $\sin\theta_7 = 0$, which implies that $Z_7^2 = |Z_7|^2$. In this case, assuming $Z_5 \equiv |Z_5|e^{i\theta_5} \neq 0$, it follows that

$$\cos\theta_5 = \frac{\text{Re}(Z_5^*Z_7^2)}{|Z_5||Z_7|^2}, \quad \sin\theta_5 = -\frac{\text{Im}(Z_5^*Z_7^2)}{|Z_5||Z_7|^2}, \quad (119)$$

in the case of $Z_6 = 0$.

Hence,

$$e^{2i\theta_{23}} = \frac{|Z_5|e^{i\theta_5}}{Z_5e^{-2i\theta_{23}}}, \quad (120)$$

where the numerator and denominator on the right-hand side of Eq. (120) are evaluated by employing Eqs. (119) and (49), respectively. Taking the square root of Eq. (120) determines θ_{23} modulo π .

If $Z_5 = Z_6 = 0$, then the squared-mass matrix of the neutral Higgs scalars is diagonal. In this case, the mass basis and the Higgs basis (with Z_7 real) coincide and the scalar potential and vacuum are CP conserving.

The case of $Z_{67} = 0$ must be separately considered. If $Z_{67} = 0$ and $Z_1 \neq Z_2$, then as discussed below Eq. (89), it follows that $Z_6 = Z_7 = 0$ corresponding to the IDM. The exceptional region of parameter space corresponding to $Z_{67} = 0$, $Z_6 \neq 0$, and $Z_1 = Z_2$ is treated in Appendix B. In this case, Eq. (78) is replaced by

$$e^{i\xi} = e^{i\xi'}e^{-i\theta_6}, \quad (121)$$

where $Z_6 \equiv |Z_6|e^{i\theta_6}$ and $\xi' \equiv \xi + \theta_6$ is a pseudoinvariant quantity that is determined modulo π in Appendix B. Once again, we see that in a convention where $\xi = 0$, the \mathbb{Z}_2 basis is uniquely defined up to a twofold ambiguity corresponding to the fact that ξ' , and hence θ_6 and θ_{23} , have been determined modulo π .

Finally, in light of the remarks at the end of Sec. IV, we can conclude that in a convention in which $\xi = 0$, once a specific discrete symmetry is chosen (among the four specified in Table II), both $\tan\beta$ and θ_{23} are promoted to physical parameters of the model.

E. An exact \mathbb{Z}_2 symmetry

In Sec. V B, we defined the \mathbb{Z}_2 basis to be the scalar basis in which $\lambda_6 = \lambda_7 = 0$. If in addition $m_{12}^2 = 0$ in the same basis, then the scalar potential possesses an exact \mathbb{Z}_2 symmetry; i.e., it is invariant under $\Phi_1 \rightarrow \Phi_1$ and $\Phi_2 \rightarrow -\Phi_2$. In this case, the condition $m_{12}^2 = 0$ yields additional constraints. In light of Eq. (A20),

$$\frac{1}{2}(Y_2 - Y_1)s_{2\beta} - \text{Re}(Y_3e^{i\xi})c_{2\beta} - i\text{Im}(Y_3e^{i\xi}) = 0, \quad (122)$$

where ξ and β have been determined previously by Eqs. (78) and (81), respectively, under the assumption that $Z_{67} \neq 0$. Hence, employing $e^{i\xi} = \pm e^{-i\theta_{67}} = \pm Z_{67}^*/|Z_{67}|$ in Eq. (122), it follows that

$$(Y_2 - Y_1)|Z_{67}|^2 - (Z_2 - Z_1)\text{Re}(Y_3Z_{67}^*) = 0, \quad (123)$$

$$\text{Im}(Y_3Z_{67}^*) = 0. \quad (124)$$

Due to Eq. (124), one can replace $\text{Re}(Y_3Z_{67}^*)$ in Eq. (123) by $Y_3Z_{67}^*$ and then divide the resulting equation by Z_{67}^* . It follows that for $Z_{67} \neq 0$, one can replace Eq. (123) by

$$(Y_2 - Y_1)Z_{67} - Y_3(Z_2 - Z_1) = 0. \quad (125)$$

The analysis above relied on the assumption that $Z_{67} \neq 0$. Thus, we now examine the relevant conditions for an exactly \mathbb{Z}_2 -symmetric scalar potential when $Z_{67} = 0$.

If $Z_{67} = 0$ and $Z_6 = 0$, then we also have $Z_7 = Y_3 = 0$ [the latter of Eq. (24)], in which case the exact \mathbb{Z}_2 symmetry is manifest in the Higgs basis. Consequently, in what follows, we shall assume that $Z_{67} = 0$ and $Z_6 \neq 0$.

If $Z_{67} = 0$ and $Z_1 \neq Z_2$, then Eq. (70) implies that $s_{2\beta} = 0$, in which case Eq. (122) yields $\text{Re}(Y_3 e^{i\xi}) = \text{Im}(Y_3 e^{i\xi}) = 0$. That is, $Y_3 = 0$, and we again conclude that $Z_6 = Z_7 = 0$ in light of Eq. (24), which reduces to the previous case considered.

If $Z_{67} = 0$, $Y_1 = Y_2$, and $Z_1 = Z_2$, then it follows from Eqs. (24) and (122) that $\beta = \frac{1}{4}\pi$ and $\text{Im}(Z_6 e^{i\xi}) = 0$. The real part of Eq. (71) then yields $\text{Re}(Z_6 e^{i\xi}) = 0$, which implies $Z_6 = 0$, which again reduces to the previous case considered.

In the three subcases considered above, Eq. (125) remains valid. However, there is one last case where Eq. (125) is trivially satisfied and yet an additional constraint must be imposed in order to achieve a \mathbb{Z}_2 -symmetric scalar potential. Consider the case of $Z_{67} = 0$, $Y_1 \neq Y_2$, $Z_1 = Z_2$, and $Z_6 \neq 0$. In this case, ξ and β are determined from Eq. (122) [since Eq. (70) is no longer relevant]. We first note that the imaginary part of Eq. (122) yields $\text{Im}(Z_6 e^{i\xi}) = 0$ after employing Eq. (24). Denoting $Z_6 \equiv |Z_6| e^{i\theta_6}$, it follows that $\xi + \theta_6 = n\pi$, for some integer n . Hence, $e^{i\xi} = \pm e^{-i\theta_6} = \pm Z_6^*/|Z_6|$, which when applied in Eqs. (71) and (122) yields

$$\frac{1}{2} s_{2\beta} (Y_2 - Y_1) |Z_6| \mp \text{Re}(Y_3 Z_6^*) c_{2\beta} \mp i \text{Im}(Y_3 Z_6^*) = 0, \quad (126)$$

$$s_{2\beta} c_{2\beta} [(Z_1 - Z_{34}) |Z_6|^2 - \text{Re}(Z_5^* Z_6^2)] + i s_{2\beta} \text{Im}(Z_5^* Z_6^2) \pm 2 c_{4\beta} |Z_6|^3 = 0. \quad (127)$$

In light of $Y_3 = -\frac{1}{2} Z_6 v^2$, Eq. (126) yields

$$\tan 2\beta = \frac{s_{2\beta}}{c_{2\beta}} = \pm \frac{v^2 |Z_6|}{Y_1 - Y_2}. \quad (128)$$

Since $Z_6 \neq 0$, it follows that $s_{2\beta} \neq 0$. Hence, the imaginary part of Eq. (127) yields

$$\text{Im}(Z_5^* Z_6^2) = 0. \quad (129)$$

Dividing the real part of Eq. (127) by $s_{2\beta}^2$ and using the result of Eq. (128), we end up with

$$v^2 (Y_1 - Y_2) [(Z_1 - Z_{34}) |Z_6|^2 - \text{Re}(Z_5^* Z_6^2)] + 2 |Z_6|^2 [(Y_1 - Y_2)^2 - v^4 |Z_6|^2] = 0. \quad (130)$$

We can replace Eqs. (129) and (130) by a single complex equation by multiplying Eq. (129) by $-iv^2(Y_1 - Y_2)$ and adding the result to Eq. (130). Additional simplification ensues by using Eq. (24) to put $|Z_6|^2(Z_1 v^2 + 2Y_1) = 0$. It then follows that

$$(Y_1 - Y_2) \left[|Z_6|^2 \left(Z_{34} + \frac{2Y_2}{v^2} \right) + Z_5^* Z_6^2 \right] + 2 |Z_6|^4 v^2 = 0. \quad (131)$$

In conclusion, Eqs. (89) and (125) are necessary conditions for the presence of an exact \mathbb{Z}_2 symmetry. These are also sufficient conditions in all cases with two exceptions. As previously noted, if $Z_1 = Z_2$, $Z_{67} \neq 0$ and $Z_5 \neq 0$, then Eq. (89) must be supplemented with the additional constraint of $\text{Im}(Z_5^* Z_6^2) = 0$. In addition, if $Z_1 = Z_2$, $Z_{67} = 0$, $Y_1 \neq Y_2$, and $Z_6 \neq 0$, then Eq. (125) must be supplemented by Eq. (131).

In this paper, we are primarily interested in the case where either the scalar potential or the vacuum is CP violating. However, it is easy to see that if the \mathbb{Z}_2 symmetry is exact, then both the scalar potential and vacuum are CP conserving. In the \mathbb{Z}_2 basis, since $m_{12}^2 = \lambda_6 = \lambda_7 = 0$, the only potentially complex scalar potential parameter is λ_5 , whose phase can be removed by an appropriate rephasing of the Higgs fields. Moreover, if $\langle \Phi_1^\dagger \Phi_2 \rangle = \frac{1}{2} v_1 v_2 e^{i\xi}$, then the ξ -dependent term of the scalar potential is of the form $\mathcal{V} \ni \frac{1}{4} \lambda_5 v_1^2 v_2^2 \cos 2\xi$, which is minimized when $\xi = 0, \frac{1}{2}\pi$ or π (depending on the sign of λ). If $\xi = \frac{1}{2}\pi$, then one can rephase $\Phi_2 \rightarrow i\Phi_2$, which simply changes the sign λ_5 while rendering the two vevs relatively real. Hence, the vacuum is CP conserving. Having achieved a scalar potential with only real parameters and real vevs, it immediately follows that a real Higgs basis exists. That is, a Higgs basis exists such that Z_5, Z_6 , and Z_7 (and $Y_3 = -\frac{1}{2} Z_6 v^2$ via the scalar potential minimum condition) are simultaneously real.

Nevertheless, it is instructive to show directly that the existence of a real Higgs basis can be deduced solely from the relations satisfied by the Higgs basis parameters when an exact \mathbb{Z}_2 symmetry is present. First, consider the case where the exact \mathbb{Z}_2 symmetry is manifest in the Higgs basis, i.e., $Y_3 = Z_6 = Z_7 = 0$. In this case, the only potentially complex parameter in the Higgs basis is Z_5 . The phase of Z_5 can be removed by a rephasing of the Higgs basis field H_2 . Hence, if the \mathbb{Z}_2 symmetry is manifest in the Higgs basis, then a real Higgs basis exists and the scalar potential and the vacuum are CP conserving.

Next, suppose that $Z_{67} \neq 0$. Then, if we combine Eqs. (88) and (124) and employ the scalar potential minimum condition, it follows that if the \mathbb{Z}_2 symmetry is exact, then

$$\text{Im}(Z_5^* Z_6^2) = \text{Im}(Z_6^* Z_7) = 0. \quad (132)$$

Given that $Z_{67} \neq 0$, the two conditions exhibited in Eq. (132) are sufficient to guarantee the existence of a real Higgs basis in which Z_5, Z_6 , and Z_7 are simultaneously real. If $Z_{67} = 0$ and $Z_1 \neq Z_2$, then Eq. (87) implies that $Z_6 = Z_7 = 0$ in which case the \mathbb{Z}_2 symmetry is manifest in the Higgs basis and the previous considerations apply. Finally, if $Z_{67} = 0$, $Z_6 \neq 0$, and $Z_1 = Z_2$, then Eq. (129) implies the existence of a real Higgs basis. Thus, in all possible cases, if an exact \mathbb{Z}_2 symmetry is present in some scalar field basis, then a real Higgs basis exists and the scalar potential and vacuum in any scalar basis are CP conserving.

If the \mathbb{Z}_2 symmetry is exact, then a real Higgs basis exists, and the Higgs basis parameters in Eq. (123) can be taken to be real. Employing Eq. (24) then yields

$$\frac{2Y_2}{v^2}(Z_6 + Z_7) + Z_1Z_7 + Z_2Z_6 = 0. \quad (133)$$

Equations (90) and (133) are equivalent to eqs. (18) and (19) of Ref. [46]. Note that Eq. (133) is trivially satisfied if $Z_{67} = 0$ and $Z_1 = Z_2$. In this latter case, one must also impose Eq. (131) to guarantee the presence of an exact \mathbb{Z}_2 symmetry. This last observation was missed in Ref. [46].

VI. THE C2HDM IN THE \mathbb{Z}_2 BASIS

The C2HDM is a two-Higgs-doublet model in which either the scalar potential or the vacuum is CP violating. To avoid tree-level Higgs-mediated FCNCs, one imposes a \mathbb{Z}_2 symmetry on the dimension-four terms of the Higgs Lagrangian. The symmetry is manifest in the Φ basis by setting $\lambda_6 = \lambda_7 = 0$ in Eq. (2). The \mathbb{Z}_2 symmetry is assumed to be softly broken by taking $m_{12}^2 \neq 0$. If the CP violation in the scalar potential is explicit, then $\text{Im}(\lambda_5^*[m_{12}^2]^2) \neq 0$. Imposing the \mathbb{Z}_2 symmetry on Eq. (53) implies that the Higgs-quark Yukawa couplings are either of Type I or Type II as discussed in Sec. IV.

In Sec. V D, we noted that one is always free to rephase the Higgs-doublet fields such that the vevs are real. (The corresponding results prior to rephasing the vevs are given in Appendix E.) Henceforth, we define the C2HDM in the \mathbb{Z}_2 basis such that $\xi = \arg(v_1^*v_2) = 0$. That is,

$$\sqrt{2}\langle\Phi_1^0\rangle \equiv v_1 = vc_\beta, \quad \sqrt{2}\langle\Phi_2^0\rangle \equiv v_2 = vs_\beta, \quad (134)$$

in the notation of Eqs. (3) and (4), where $c_\beta \equiv \cos\beta$ and $s_\beta \equiv \sin\beta$, with $0 \leq \beta \leq \frac{1}{2}\pi$. In this convention, one may parametrize the scalar doublets in the Φ basis as

$$\begin{aligned} \Phi_1 &= \begin{pmatrix} \varphi_1^+ \\ \frac{1}{\sqrt{2}}(v_1 + \eta_1 + i\chi_1) \end{pmatrix}, \\ \Phi_2 &= \begin{pmatrix} \varphi_2^+ \\ \frac{1}{\sqrt{2}}(v_2 + \eta_2 + i\chi_2) \end{pmatrix}. \end{aligned} \quad (135)$$

Setting $\lambda_6 = \lambda_7 = \xi = 0$ in Eq. (E3) yields the C2HDM scalar potential minimum conditions,

$$m_{11}^2 = \text{Re } m_{12}^2 \tan\beta - \frac{1}{2}v^2[\lambda_1c_\beta^2 + (\lambda_3 + \lambda_4 + \text{Re } \lambda_5)s_\beta^2], \quad (136)$$

$$m_{22}^2 = \text{Re } m_{12}^2 \cot\beta - \frac{1}{2}v^2[\lambda_2s_\beta^2 + (\lambda_3 + \lambda_4 + \text{Re } \lambda_5)c_\beta^2], \quad (137)$$

$$\text{Im } m_{12}^2 = \frac{1}{2}v^2s_\beta c_\beta \text{Im } \lambda_5. \quad (138)$$

After eliminating m_{12}^2 , m_{22}^2 , and $\text{Im } m_{12}^2$, we are left with nine real parameters that govern the C2HDM: v , $\tan\beta$, $\text{Re } m_{12}^2$, λ_1 , λ_2 , λ_3 , λ_4 , $\text{Re } \lambda_5$, and $\text{Im } \lambda_5$. By adopting the convention where both vevs are real and positive, it follows that if $s_{2\beta} \neq 0$ and $\text{Im } \lambda_5 \neq 0$ [which implies that $\text{Im } m_{12}^2 \neq 0$ via Eq. (138)], then CP is violated in the scalar sector.

If CP is violated in the scalar sector, then the violation is either explicit or spontaneous. A scalar potential of the 2HDM is explicitly CP conserving if and only if a real basis exists [59] (i.e., a basis of scalar fields exists in which all the scalar potential parameters are real). However, in transforming to a real basis, the vevs (which were real in the original basis by convention) may acquire a relative complex phase that is unremovable by any further basis change that maintains the reality of the scalar field basis. This latter scenario corresponds to the case of spontaneous CP violation. Consequently, both spontaneous and explicit CP violation are treated simultaneously in the convention adopted in Eq. (134).

It is instructive to perform the counting of parameters using the invariants quantities discussed in previous sections. After employing Eq. (24), one is left initially with six real parameters, v , Y_2 , Z_1 , Z_2 , Z_3 , and Z_4 , and three complex parameters, Z_5 , Z_6 , and Z_7 , for a total of 12 parameters. Since one can rephase the pseudoinvariant Higgs basis field H_2 , this freedom removes one phase from the three complex parameters. Finally, since a softly broken \mathbb{Z}_2 symmetry is present, one obtains one complex constraint equation (derived in Sec. V) that removes two additional parameters. This leaves nine independent real parameters in agreement with our previous counting.

If $s_{2\beta} = 0$, then the model corresponds to the IDM which is CP conserving. Consequently, in our considerations of the C2HDM, we shall henceforth assume that $s_{2\beta} \neq 0$, which is a necessary ingredient for the presence of CP violation, as noted below Eq. (138). Since $\lambda_6 = \lambda_7 = 0$ (in the \mathbb{Z}_2 basis), it then follows from Eq. (D1) that if $\lambda_1 \neq \lambda_2$, then $\lambda_6 + \lambda_7$ is nonzero when evaluated in any other scalar field basis. In particular, $\lambda_1 \neq \lambda_2$ implies that $Z_{67} \neq 0$. In contrast, if $\lambda_1 = \lambda_2$ in the \mathbb{Z}_2 basis, then it

follows that $Z_1 = Z_2$ and $Z_{67} = 0$, which corresponds to the exceptional region of the parameter space (see Appendix B).

In light of Eqs. (21), (25), and (31), one can identify the massless would-be neutral Goldstone boson with $G^0 = c_\beta \chi_1 + s_\beta \chi_2$. Thus, the neutral scalar state orthogonal to G^0 is

$$\eta_3 = -s_\beta \chi_1 + c_\beta \chi_2. \quad (139)$$

After diagonalizing the squared-mass matrix of the neutral scalar fields, η_1 , η_2 , and η_3 , the three neutral mass-eigenstate scalar fields, h_1 , h_2 , and h_3 , can be identified as

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \mathcal{R} \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix}. \quad (140)$$

In the C2HDM literature, the 3×3 orthogonal mixing matrix \mathcal{R} is parametrized as [60]

$$\mathcal{R} = \begin{pmatrix} c_1 c_2 & s_1 c_2 & s_2 \\ -c_1 s_2 s_3 - s_1 c_3 & c_1 c_3 - s_1 s_2 s_3 & c_2 s_3 \\ -c_1 s_2 c_3 + s_1 s_3 & -c_1 s_3 - s_1 s_2 c_3 & c_2 c_3 \end{pmatrix}, \quad (141)$$

where $s_i = \sin \alpha_i$ and $c_i = \cos \alpha_i$ ($i = 1, 2, 3$).

It is now straightforward to relate the angles α_1 , α_2 , and α_3 of the C2HDM literature to basis-independent quantities introduced in Sec. II. In Appendix E, we have examined the mixing of the neutral scalars in the \mathbb{Z}_2 basis. Setting $\xi = 0$ in Eqs. (E9)–(E11) yields

$$\mathcal{R}_{k1} = q_{k1} c_\beta - \text{Re}(q_{k2} e^{-i\theta_{23}}) s_\beta, \quad (142)$$

$$\mathcal{R}_{k2} = q_{k1} s_\beta + \text{Re}(q_{k2} e^{-i\theta_{23}}) c_\beta, \quad (143)$$

$$\mathcal{R}_{k3} = \text{Im}(q_{k2} e^{-i\theta_{23}}). \quad (144)$$

One can relate the mixing angles α_1 , α_2 , and α_3 to invariant (or pseudoinvariant) quantities by setting $\xi = 0$ in Eqs. (E12) and (E13). It is convenient to define $\bar{\alpha}_1 \equiv \alpha_1 - \beta$. We then obtain the results exhibited in Table III.

In the presence of a softly broken \mathbb{Z}_2 symmetry, Eq. (75) implies that the quantity $e^{i(\xi + \theta_{23})}$ is determined up to a twofold ambiguity associated with a residual basis dependence corresponding to the interchange of the two scalar doublets while maintaining $\lambda_6 = \lambda_7 = 0$. Having adopted the C2HDM convention where $\xi = 0$, it therefore follows that $e^{i\theta_{23}}$ is determined up to a twofold ambiguity. In particular, one no longer has the freedom to rephase the Higgs basis field H_2 , which would result in an additive shift of the parameter θ_{23} [cf. Eq. (39)]. In light of Eqs. (72)–(75), it follows that under the basis transformation that simply

TABLE III. The relation between the neutral Higgs mixing angles α_i of the C2HDM defined in the \mathbb{Z}_2 basis and (pseudo)-invariant combinations of mixing angles defined in the Higgs basis. In the notation used below, $\bar{c}_1 \equiv \cos \bar{\alpha}_1$ and $\bar{s}_1 \equiv \sin \bar{\alpha}_1$, with $\bar{\alpha}_1 \equiv \alpha_1 - \beta$.

k	q_{k1}	$q_{k2} e^{-i\theta_{23}}$
1	$\bar{c}_1 c_2$	$\bar{s}_1 c_2 + i s_2$
2	$-\bar{c}_1 s_2 s_3 - \bar{s}_1 c_3$	$\bar{c}_1 c_3 - \bar{s}_1 s_2 s_3 + i c_2 s_3$
3	$-\bar{c}_1 s_2 c_3 + \bar{s}_1 s_3$	$-\bar{c}_1 s_3 - \bar{s}_1 s_2 c_3 + i c_2 c_3$

interchanges Φ_1 and Φ_2 (with no rephasing), $s_\beta \leftrightarrow c_\beta$ and $e^{i\theta_{23}} \rightarrow -e^{i\theta_{23}}$. Moreover,

$$\begin{aligned} s_1 &\rightarrow c_1, & c_1 &\rightarrow s_1, & s_2 &\rightarrow -s_2, \\ c_2 &\rightarrow c_2, & s_3 &\rightarrow -s_3, & c_3 &\rightarrow -c_3, \end{aligned} \quad (145)$$

which yields $\mathcal{R}_{k1} \leftrightarrow \mathcal{R}_{k2}$ and $\mathcal{R}_{k3} \rightarrow -\mathcal{R}_{k3}$. These results are consistent with Eqs. (142)–(144) since the q_{k1} and q_{k2} are basis-invariant quantities.

Finally, we note that the free parameter $\text{Re} m_{12}^2$ can also be related to basis-invariant quantities by employing Eq. (A20) with $\xi = 0$ and Eq. (24), and making use of the results of Sec. V D. If $\lambda_1 \neq \lambda_2$, then $Z_{67} \neq 0$, in which case Eqs. (110) and (111) yield

$$\begin{aligned} \text{Re} m_{12}^2 &= \frac{1}{4} v^2 s_{2\beta} \left[Z_1 + \frac{2Y_2}{v^2} \right. \\ &\quad \left. - \left(\frac{|Z_6|^2 + \text{Re}(Z_6 Z_7^*)}{|Z_{67}|^2} \right) (Z_1 - Z_2) \right], \end{aligned} \quad (146)$$

where $s_{2\beta}$ is given by Eq. (82). The case of $\lambda_1 = \lambda_2$ in the \mathbb{Z}_2 basis corresponds to the exceptional region of parameter space, where $Z_1 = Z_2$ and $Z_{67} = 0$, as previously noted. In this case, Eq. (146) does not apply and one must employ the results of Appendix B. The resulting expression for $\text{Re} m_{12}^2$ is unwieldy and we do not present it here.

It is instructive to identify the nine real parameters of the C2HDM in terms of the scalar masses and mixing angles. In order to perform the correct counting, we note the following sum rule:

$$\sum_k m_k^2 \mathcal{R}_{k3} (\mathcal{R}_{k1} c_\beta - \mathcal{R}_{k2} s_\beta) = 0, \quad (147)$$

which is derived at the end of Appendix E. This sum rule imposes one relation among the ten real quantities, v , $\tan \beta$, α_1 , α_2 , α_3 , m_1 , m_2 , m_3 , $\text{Re} m_{12}^2$, and m_{H^\pm} , resulting in nine independent parameters. One can repeat the counting of parameters using basis-invariant quantities. In light of Eq. (40) and Eqs. (47)–(50), one can eliminate Z_1 , Z_3 , Z_4 , $Z_5 e^{-2i\theta_{23}}$, and $Z_6 e^{-i\theta_{23}}$ in terms of scalar masses and the invariant mixing angles θ_{12} and θ_{13} . This leaves three

invariant parameters, Z_2 , $\text{Re}(Z_7 e^{-i\theta_{23}})$ and $\text{Im}(Z_7 e^{-i\theta_{23}})$, of which two are determined from the one complex constraint equation arising from the condition of a softly broken \mathbb{Z}_2 symmetry. For example, if we eliminate the complex parameter Z_7 using Eq. (89), we are left with the following nine real parameters: v , Y_2 , Z_2 , θ_{12} , θ_{13} , m_1 , m_2 , m_3 , and m_{H^\pm} .

The complete set of Feynman rules for the C2HDM in terms of the \mathbb{Z}_2 -basis parameters can be found in Refs. [32,61]. One can check that all the Higgs couplings obtained this way (after using Eq. (41) to define an invariant charged Higgs field) are invariant with respect to basis transformations. As previously noted, all the bosonic couplings of the most general 2HDM (without any imposed discrete symmetries) can be found in Ref. [34] expressed directly in terms of invariant quantities q_{k1} , q_{k2} , and the Higgs basis scalar potential coefficients (including appropriate factors of $e^{-i\theta_{23}}$ to ensure basis-independent combinations). The bosonic couplings of the most general 2HDM also apply to the C2HDM, since as emphasized in Sec. V, $\tan\beta$ does not appear explicitly in any of these couplings. It is a straightforward to verify that the cubic and quartic Higgs self-couplings, which appear in Ref. [34], match precisely the corresponding C2HDM couplings given in Ref. [61].

Finally, the Type-Ia and Type-IIa Higgs-quark couplings are obtained from Eq. (58) by employing Eqs. (65) and (67) with $\xi = 0$ [in the convention of Eq. (134)]. For example,¹²

$$\begin{aligned}
-\mathcal{L}_{\text{Type-Ia}} = & \frac{1}{v} \{ \bar{U} M_U [q_{k1} + \text{Re}(q_{k2} e^{-i\theta_{23}}) \cot\beta \\
& - i\gamma_5 \text{Im}(q_{k2} e^{-i\theta_{23}}) \cot\beta] U h_k \\
& + \bar{D} M_D [q_{k1} + \text{Re}(q_{k2} e^{-i\theta_{23}}) \cot\beta \\
& + i\gamma_5 \text{Im}(q_{k2} e^{-i\theta_{23}}) \cot\beta] D h_k \},
\end{aligned} \tag{148}$$

$$\begin{aligned}
-\mathcal{L}_{\text{Type-IIa}} = & \frac{1}{v} \{ \bar{U} M_U [q_{k1} + \text{Re}(q_{k2} e^{-i\theta_{23}}) \cot\beta \\
& - i\gamma_5 \text{Im}(q_{k2} e^{-i\theta_{23}}) \cot\beta] U h_k \\
& + \bar{D} M_D [q_{k1} - \text{Re}(q_{k2} e^{-i\theta_{23}}) \tan\beta \\
& - i\gamma_5 \text{Im}(q_{k2} e^{-i\theta_{23}}) \tan\beta] D h_k \},
\end{aligned} \tag{149}$$

where there is an implicit sum over the three neutral Higgs mass-eigenstates h_k . Using the results of Table III, one can reproduce the results of Ref. [32]. Indeed, as previously noted, $\tan\beta$ and $e^{-i\theta_{23}}$ now appear explicitly in the Yukawa couplings. However, these quantities are not quite physical parameters, since under the basis change $\Phi_1 \leftrightarrow \Phi_2$, it

follows that $\cot\beta \leftrightarrow \tan\beta$ and $e^{-i\theta_{23}}$ change sign. This has the effect of interchanging the a and b versions of the Type-I and Type-II Yukawa couplings (cf. footnote 12).

In order to promote $\tan\beta$ and $e^{i\theta_{23}}$ to physical parameters, one must remove the remaining freedom to interchange $\Phi_1 \leftrightarrow \Phi_2$ in the C2HDM. This corresponds to making a specific choice of the discrete symmetry among the four specified in Table II. In practice, this can be achieved by declaring, e.g., that $\tan\beta < 1$ corresponds to an *enhanced* coupling of the neutral Higgs bosons to up-time quarks. Given this additional proviso, it follows that the signs of $c_{2\beta}$ and $e^{i\theta_{23}}$ are then fixed and can now be considered as physical parameters of the model. Indeed, $c_{2\beta}$ can be expressed in terms of basis-invariant parameters as specified in Eq. (82), where the sign ambiguity is fixed by the sign of $\lambda_1 - \lambda_2$ [cf. Eq. (A16)], under the assumption that $\lambda_1 \neq \lambda_2$. Likewise, $e^{i\theta_{23}}$ is uniquely determined by the formal basis-independent expression given by Eq. (116) [after employing Eq. (82) for $s_{2\beta}/c_{2\beta}$ with the sign ambiguity fixed as indicated above]. Finally, the exceptional region of the parameter space where $\lambda_1 = \lambda_2$ in the \mathbb{Z}_2 basis is treated in Appendix B.

VII. DETECTING DISCRETE SYMMETRIES

In Ref. [46], Lavoura described ways to detect the presence of discrete symmetries exhibited by the scalar potential of the 2HDM. Four cases of discrete symmetries were examined: (i) exact \mathbb{Z}_2 symmetry; (ii) explicit CP breaking by a complex soft \mathbb{Z}_2 -breaking squared-mass term (which defines the C2HDM); (iii) softly broken \mathbb{Z}_2 and spontaneously broken CP symmetries [62]; and (iv) the Lee model of spontaneous CP violation [1], where no (unbroken or softly broken) \mathbb{Z}_2 symmetry is present. For the reader's convenience, we provide a translation between Lavoura's notation and the notation of this paper,

$$\begin{aligned}
\lambda_1, \lambda_2, \lambda_5 & \longrightarrow \frac{1}{2} Z_1, \frac{1}{2} Z_2, \frac{1}{2} Z_5, \\
\lambda_3, \lambda_4, \lambda_6, \lambda_7 & \longrightarrow Z_3, Z_4, Z_6, Z_7, \\
\mu_1, \mu_2, \mu_3 & \longrightarrow Y_1, Y_2, Y_3, \quad v \longrightarrow v/\sqrt{2}.
\end{aligned} \tag{150}$$

In case (i), Lavoura asserts that Eqs. (18) and (19) of Ref. [46] are the conditions for an exact \mathbb{Z}_2 -symmetric scalar potential. We have confirmed that these conditions are both necessary and sufficient in Sec. V E, as indicated below Eq. (133).

In case (ii), Lavoura asserts that Eqs. (20) and (21) of Ref. [46] are the conditions for explicit CP breaking by a complex soft \mathbb{Z}_2 -breaking term. We have confirmed that these results are a consequence of Eqs. (87) and (88). Indeed, Eq. (88) is equivalent to eq. (20) of Ref. [46]. In addition, by multiplying Eq. (89) by $Z_6 - Z_7$ and then taking the imaginary part of the resulting expression, one reproduces eq. (21) of Ref. [46],

¹²As discussed in Sec. IV, the Yukawa couplings for Type Ib and IIb can be obtained from Eqs. (148) and (149), respectively, by replacing $\cot\beta \leftrightarrow \tan\beta$ and changing the sign of $e^{-i\theta_{23}}$.

$$(Z_1 - Z_2)\text{Im}[Z_5^*(Z_6^2 - Z_7^2)] - [(Z_1 - Z_2)(Z_1 + Z_2 - 2Z_{34}) + 4(|Z_6|^2 - |Z_7|^2)]\text{Im}(Z_6Z_7^*) = 0. \quad (151)$$

In case (iii), Lavoura asserts that Eqs. (20)–(22) of Ref. [46] are the conditions for a softly broken Z_2 -symmetric scalar potential and spontaneously broken CP symmetry. We have confirmed Lavoura's results in Sec. V C, while noting a typographical error in eq. (22) of Ref. [46] (see footnote 9). The corresponding corrected equation (with a different overall normalization) was given in Eq. (103). Moreover, Lavoura's results are not applicable in cases of $Z_1 = Z_2$ and/or $Z_{67} = 0$. The correct expressions that replace Eq. (103) in these special cases have been obtained in Sec. V C and Appendix B. Note that if $Z_6 \neq \pm Z_7$, then only two of the three equations among Eqs. (87), (88), and (151) are independent.¹³

In case (iv), Lavoura attempts to discover the conditions on the 2HDM Higgs basis parameters that govern the Lee model of spontaneous CP violation [1]. In this model, the Z_2 symmetry is absent, i.e., there is no basis of scalar fields in which $\lambda_6 = \lambda_7 = 0$. A scalar field basis exists in the Lee model in which all the scalar potential parameters are simultaneously real, implying that the scalar potential is explicitly CP conserving. However, there is an unremovable relative complex phase between the two vevs $\langle \Phi_1^0 \rangle$ and $\langle \Phi_2^0 \rangle$. Moreover, no real Higgs basis exists. In terms of the Higgs basis parameters, the nonexistence of a real Higgs basis implies that at least one of the following three quantities, $\text{Im}(Z_6^2Z_5^*)$, $\text{Im}(Z_7^2Z_5^*)$, and $\text{Im}(Z_6Z_7^*)$ must be nonvanishing [cf. Eq. (30)]. Hence, the vacuum is CP violating; that is, the Lee model exhibits spontaneous CP violation.

When considering the Lee model, Lavoura noted in Ref. [46] that there should be two relations among the parameters of the Lee model, corresponding to the two independent CP-odd invariants. Lavoura found one relation, that appears in eq. (27) of Ref. [46]. But he was unable to identify the second invariant condition. We now proceed to confirm Lavoura's invariant quantity and to complete his mission by finding the second invariant quantity that was missed. Moreover, we shall demonstrate that in certain regions of the parameter space of the Lee model, Lavoura's invariant vanishes, in which case two additional invariant quantities must be introduced in order to cover all possible special cases.

Consider the scalar potential of the general 2HDM given in Eq. (2), with no constraints initially imposed on the scalar potential parameters. To check for the presence of explicit CP violation in all possible regions of the 2HDM parameter space, it is necessary and sufficient to consider

¹³Note that $\text{Im}[(Z_6 + Z_7)E] = 0$ yields Eq. (88) and $\text{Im}[(Z_6 - Z_7)E] = 0$ yields Eq. (151), where E denotes the left-hand side of Eq. (89). It then follows that $\text{Re}[(Z_6 + Z_7)E] = 0$, which is equivalent to Eq. (87).

four CP-odd basis-invariant quantities, identified in Ref. [59], as follows¹⁴:

$$I_{Y3Z} \equiv \text{Im}(Z_{a\bar{c}}^{(1)}Z_{e\bar{b}}^{(1)}Z_{b\bar{c}\bar{d}}Y_{d\bar{a}}), \quad (152)$$

$$I_{2Y2Z} \equiv \text{Im}(Y_{a\bar{b}}Y_{c\bar{d}}Z_{b\bar{a}\bar{d}\bar{f}}Z_{f\bar{c}}^{(1)}), \quad (153)$$

$$I_{6Z} \equiv \text{Im}(Z_{a\bar{b}\bar{c}\bar{d}}Z_{b\bar{f}}^{(1)}Z_{d\bar{h}}^{(1)}Z_{f\bar{a}\bar{j}\bar{k}}Z_{k\bar{j}\bar{m}\bar{n}}Z_{n\bar{m}\bar{h}\bar{c}}), \quad (154)$$

$$I_{3Y3Z} \equiv \text{Im}(Z_{a\bar{c}\bar{b}\bar{d}}Z_{c\bar{e}\bar{d}\bar{g}}Z_{e\bar{h}\bar{f}\bar{q}}Y_{g\bar{a}}Y_{h\bar{b}}Y_{q\bar{f}}). \quad (155)$$

If all four of these CP-odd invariants vanish, then there exists a real Φ basis, in which case the scalar potential is *explicitly* CP conserving. Aside from special regions in parameter space, at most two of these invariants are independent, as we will demonstrate below.

Explicit forms for the above four CP-odd invariants can be found in Ref. [59]. We proceed to evaluate them in the Higgs basis. After employing Eq. (24), it follows that

$$I_{Y3Z} = \frac{1}{2}v^2 \left\{ 2f_2f_3 + (Z_1 - Z_2)[\text{Im}(Z_5^*Z_6Z_{67}) - (Z_1 - Z_{34})f_3] - \left(Z_1 + \frac{2Y_2}{v^2} \right) [\text{Im}(Z_5^*Z_6^2) - (Z_1 - Z_2)f_3] \right\}, \quad (156)$$

$$I_{2Y2Z} = \frac{1}{4}v^4 \left\{ (Z_1 - Z_2)\text{Im}(Z_5^*Z_6^2) - \left(Z_1 + \frac{2Y_2}{v^2} \right) [(Z_1 - Z_{34})f_3 + \text{Im}(Z_5^*Z_6Z_{67})], + \left[\left(Z_1 + \frac{2Y_2}{v^2} \right)^2 - 2|Z_6|^2 + 2\text{Re}(Z_6Z_7^*) \right] f_3 \right\}, \quad (157)$$

where the f_i are defined in Eq. (95). One can check that $-I_{Y3Z}/v^2$ corresponds precisely to the left-hand side of eq. (27) of Ref. [46]. Thus, I_{2Y2Z} is the second invariant quantity that governs the Lee model, which is the one that Lavoura was unable to find.

Apart from special regions of the Lee model parameter space, $I_{Y3Z} = I_{2Y2Z} = 0$ provide nontrivial relations among the parameters that must hold for a spontaneously CP-violating scalar sector. However, there exist special regions

¹⁴Three CP-odd invariants that are equivalent to Eqs. (152)–(154) were also identified in Ref. [63]. Subsequently, a group-theoretic formulation of the 2HDM scalar potential was developed in Refs. [36,37] that provided an elegant form for the basis-independent conditions governing explicit CP conservation in the 2HDM. The bilinear formalism exploited in the latter two references has also been employed in the study of the CP properties of the 2HDM scalar potential in Refs. [38–41].

of the Lee model parameter space where one or both of the invariants exhibited in Eqs. (156) and (157) automatically vanish. One such example arises in the case of a softly broken \mathbb{Z}_2 symmetry, corresponding to $\lambda_6 = \lambda_7 = 0$ in the Φ basis in which the Lee model is initially defined. This case was studied in detail in Sec. V C, where it was shown that I_{Y3Z} automatically vanishes and thus provides no constraint. Lavoura was well aware of this in Ref. [46].

Indeed, he noted that I_{Y3Z} is a linear combination of the left-hand sides of Eqs. (88) and (151). Since both of these quantities vanish if $\lambda_6 = \lambda_7 = 0$ in some scalar field basis, it follows that $I_{Y3Z} = 0$ is automatic in a model with a softly broken \mathbb{Z}_2 symmetry. One can check this explicitly as follows. First, if $Z_{67} = 0$, then $f_3 = 0$, and Eq. (156) immediately yields $I_{Y3Z} = 0$. Next, if $Z_{67} \neq 0$, then

$$\begin{aligned} \text{Im}(Z_5^* Z_6 Z_{67}) &= \frac{\text{Im}(Z_5^* Z_{67}^2 Z_6^* Z_6)}{|Z_{67}|^2} = \frac{\text{Im}(Z_5^* Z_{67}^2)[|Z_6|^2 + \text{Re}(Z_6 Z_7^*)] + \text{Re}(Z_5^* Z_{67}^2)\text{Im}(Z_6 Z_7^*)}{|Z_{67}|^2} \\ &= \frac{(f_1 - f_2)\text{Im}(Z_5^* Z_{67}^2) + 2f_3 \text{Re}(Z_5^* Z_{67}^2)}{2f_1}. \end{aligned} \quad (158)$$

Employing Eqs. (100) and (101) in Eqs. (156) and (158), one can easily verify that $I_{Y3Z} = 0$.

In Eqs. (102) and (103), an invariant condition was identified that guarantees that the scalar sector of the 2HDM with a softly broken \mathbb{Z}_2 exhibits spontaneous CP violation. We now demonstrate that this invariant condition is equivalent to the requirement that $f_3 \neq 0$ and $I_{2Y2Z} = 0$. Assuming that $Z_{67} \neq 0$, we shall make use of the following formulae:

$$\text{Im}(Z_5^* Z_6^2) = \frac{[(f_1 - f_2)^2 - 4f_3^2]\text{Im}(Z_5^* Z_{67}^2) + 4f_3(f_1 - f_2)\text{Re}(Z_5^* Z_{67}^2)}{4f_1^2}, \quad (159)$$

$$\text{Re}(Z_6 Z_7^*) - |Z_6|^2 = \frac{f_2(f_1 - f_2) - 4f_3^2}{2f_1}, \quad (160)$$

which are derived in the same manner as Eq. (158). One can now evaluate I_{2Y2Z} given in Eq. (157) with the help of Eqs. (158)–(160). Imposing the conditions of a softly broken \mathbb{Z}_2 symmetry by employing Eqs. (100) and (101), the end result of this computation is

$$I_{2Y2Z} = \frac{v^4 f_3 \mathcal{F}}{16f_1^2(Z_1 - Z_2)}, \quad (161)$$

where \mathcal{F} is given explicitly in Eq. (103). This result confirms that $f_3 \neq 0$ and $I_{2Y2Z} = 0$ are the invariant conditions for spontaneous CP violation in the softly broken \mathbb{Z}_2 -symmetric 2HDM. As discussed in Sec. V C, Eq. (161) can be used in the case of $Z_1 = Z_2$ by employing Eq. (100) to eliminate f_2 in favor of $\text{Re}(Z_5^* Z_{67}^2)$. This procedure will remove the potential singularity due to the factor of $Z_1 - Z_2$ in the denominator of Eq. (161).

Because $\lambda_6 = \lambda_7 = 0$ in the Φ basis, the only potentially nontrivial phase is the relative phase between m_{12}^2 and λ_5 . Thus, only one invariant condition is needed to determine whether or not the model exhibits spontaneous CP violation. In the special case of $Z_{67} = 0$ and $Z_1 \neq Z_2$, the conditions for a softly broken \mathbb{Z}_2 symmetry given in Eqs. (70) and (71) yield $Y_3 = Z_6 = Z_7 = 0$ [after using Eq. (24)], corresponding to the (CP-conserving) IDM

treated in Sec. V A. In the exceptional region of parameter space defined by $Z_{67} = 0$ and $Z_1 = Z_2$, it follows that $I_{2Y2Z} = 0$, and one must discover another invariant condition to determine whether the model exhibits spontaneous CP violation.

In order to exhibit cases where Eqs. (156) and (157) are not sufficient to determine whether or not the scalar potential is explicitly CP conserving, we shall make use of the observation of Ref. [59] that it is always possible to perform a basis transformation such that in the transformed basis of scalar fields, $\lambda_7 = -\lambda_6$ (a simple proof of this result is presented in Appendix D). Since basis-invariant quantities can be evaluated in any basis without changing their values, we shall evaluate the four CP-odd invariants listed in Eqs. (152)–(155) in a basis where $\lambda_7 = -\lambda_6$, where these invariants take on the following simpler forms:

$$I_{Y3Z} = (\lambda_1 - \lambda_2)^2 \text{Im}(m_{12}^2 \lambda_6^*), \quad (162)$$

$$I_{2Y2Z} = (\lambda_1 - \lambda_2)[\text{Im}(\lambda_5^* [m_{12}^2]^2) - (m_{11}^2 - m_{22}^2)\text{Im}(m_{12}^2 \lambda_6^*)], \quad (163)$$

$$I_{6Z} = -(\lambda_1 - \lambda_2)^3 \text{Im}(\lambda_6^2 \lambda_5^*), \quad (164)$$

$$\begin{aligned}
I_{3Y3Z} &= 4\text{Im}([m_{12}^2]^3(\lambda_6^*)^3) - 2\text{Im}([m_{12}^2]^3\lambda_6(\lambda_5^*)^2) \\
&\quad + [(m_{11}^2 - m_{22}^2)^2 - 6|m_{12}^2|^2](m_{11}^2 - m_{22}^2)\text{Im}(\lambda_5^*\lambda_6^2) \\
&\quad + [(\lambda_1 - \lambda_{34})(\lambda_2 - \lambda_{34}) + 2|\lambda_6|^2 - |\lambda_5|^2](m_{11}^2 - m_{22}^2)\text{Im}(\lambda_5^*[m_{12}^2]^2) \\
&\quad - \{(\lambda_1 - \lambda_2)^2 m_{11}^2 m_{22}^2 + 2(2|\lambda_6|^2 - |\lambda_5|^2)[(m_{11}^2 - m_{22}^2)^2 - |m_{12}^2|^2]\}\text{Im}(m_{12}^2\lambda_6^*) \\
&\quad - (\lambda_1 + \lambda_2 - 2\lambda_{34})\{(m_{11}^2 - m_{22}^2)\text{Im}([m_{12}^2]^2(\lambda_6^*)^2) + \text{Im}([m_{12}^2]^3\lambda_5^*\lambda_6^*) \\
&\quad - [(m_{11}^2 - m_{22}^2)^2 - |m_{12}^2|^2]\text{Im}(m_{12}^2\lambda_6\lambda_5^*)\}, \tag{165}
\end{aligned}$$

where $\lambda_{34} \equiv \lambda_3 + \lambda_4$. If $I_{Y3Z} = 0$, then additional CP-odd invariants may need to be considered.

In a Φ basis of scalar fields where $\lambda_6 = -\lambda_7$, the invariant $I_{Y3Z} = 0$ if any one of the following four conditions hold: (i) $\lambda_6 = 0$, (ii) $\lambda_1 = \lambda_2$, (iii) $m_{12}^2 = 0$, or (iv) $\text{Im}(m_{12}^2\lambda_6^*) = 0$. We now examine each of these four cases in turn. Subsequently, we shall examine two additional special cases of interest in which I_{Y3Z} does not vanish.

Case 1.— $\lambda_6 = 0$ and $\lambda_1 \neq \lambda_2$.

This case corresponds to a scalar potential with a softly broken \mathbb{Z}_2 symmetry, since $\lambda_6 = \lambda_7 = 0$ in the Φ basis. Equations (162)–(165) yield $I_{Y3Z} = I_{6Z} = 0$ and

$$I_{2Y2Z} = (\lambda_1 - \lambda_2)\text{Im}(\lambda_5^*[m_{12}^2]^2), \tag{166}$$

$$I_{3Y3Z} = \left(\frac{[(\lambda_1 - \lambda_{34})(\lambda_2 - \lambda_{34}) - |\lambda_5|^2](m_{11}^2 - m_{22}^2)}{\lambda_1 - \lambda_2} \right) I_{2Y2Z}. \tag{167}$$

The above results imply that in this case only one invariant quantity, I_{2Y2Z} , is needed to determine whether the scalar potential is explicitly CP conserving. Indeed, Eq. (166)

immediately shows that Eq. (102) is proportional to I_{2Y2Z} , a result that was obtained above by a rather tedious computation that yielded Eq. (161). Moreover, Eq. (166) provides a very simple method for computing I_{2Y2Z} in terms of Higgs basis parameters. Using Eqs. (A21) and (A22), it follows that

$$\begin{aligned}
\lambda_1 - \lambda_2 &= (Z_1 - Z_2)c_{2\beta} - 2s_{2\beta}\text{Re}(Z_{67}e^{i\xi}) \\
&= \mp \sqrt{(Z_1 - Z_2)^2 + 4|Z_{67}|^2}, \tag{168}
\end{aligned}$$

after using Eq. (82) and noting that $\text{Re}(Z_{67}e^{i\xi}) = \pm|Z_{67}|$ [cf. Eq. (78)]. Hence, by using Eqs. (102), (103), and (168) in Eq. (166), one immediately reproduces the result of Eq. (161).

Case 2.— $\lambda_1 = \lambda_2$.

In light of Eqs. (A5), (A6), (A10), and (A11), it follows that if $\lambda_1 = \lambda_2$ and $\lambda_6 = -\lambda_7$, then these relations hold in any basis of scalar fields. Hence, it follows that $Z_1 = Z_2$ and $Z_6 = -Z_7$. This is the exceptional region of the 2HDM parameter space, which is treated in more detail in Appendix B. In this case, Eqs. (162)–(165) yield $I_{Y3Z} = I_{2Y2Z} = I_{6Z} = 0$ and

$$\begin{aligned}
I_{3Y3Z} &= -\frac{1}{8}v^6\text{Im}(Z_5^*Z_6^2) \left\{ \left(Z_1 + \frac{2Y_2}{v^2} \right)^3 + 2(Z_1 - Z_{34}) \left(Z_1 + \frac{2Y_2}{v^2} \right)^2 \right. \\
&\quad \left. - [4|Z_6|^2 + |Z_5|^2 - (Z_1 - Z_{34})^2] \left(Z_1 + \frac{2Y_2}{v^2} \right) - 4[(Z_1 - Z_{34})|Z_6|^2 + \text{Re}(Z_5^*Z_6^2)] \right\}, \tag{169}
\end{aligned}$$

after evaluating I_{3Y3Z} in the Higgs basis and employing Eq. (24). If $\text{Im}(Z_5^*Z_6) = 0$, then a real Higgs basis exists and both the scalar potential and vacuum are CP conserving. If $\text{Im}(Z_5^*Z_6) \neq 0$ and $I_{3Y3Z} = 0$, then the model exhibits spontaneous CP violation. This result provides the previously missing invariant condition for spontaneous CP violation in the exceptional region of the 2HDM parameter space.

Case 3.— $m_{12}^2 = 0$, and $\lambda_1 \neq \lambda_2$.

In this case, Eqs. (162)–(165) yield $I_{Y3Z} = I_{2Y2Z} = 0$ and

$$I_{6Z} = -(\lambda_1 - \lambda_2)^3\text{Im}(\lambda_5^*\lambda_6^2), \tag{170}$$

$$I_{3Y3Z} = -\left(\frac{m_{11}^2 - m_{22}^2}{\lambda_1 - \lambda_2} \right)^3 I_{6Z}. \tag{171}$$

The above results imply that in this case only one invariant quantity, I_{6Z} , is needed to determine whether the scalar potential is explicitly CP conserving. For completeness, we provide an expression for I_{6Z} when evaluated in the Higgs basis [59],

$$\begin{aligned}
I_{6Z} = & -4f_2^2 f_3 + |Z_5|^2 \{2f_3 [f_1 - (Z_1 - Z_2)^2] + (Z_1 - Z_2) \text{Im}(Z_5^* Z_6^2 Z_7^2)\} \\
& + 2f_2 \{(Z_1 - Z_{34}) [f_3 (Z_1 - Z_2) + \text{Im}(Z_5^* Z_6^2 Z_7^2)] - (Z_1 - Z_2) \text{Im}(Z_5^* Z_6 Z_7)\} \\
& - 2f_3 (Z_1 - Z_2) \{\text{Re}(Z_5^* Z_6^2 Z_7^2) - 2\text{Re}(Z_5^* Z_6 Z_7) + (Z_1 - Z_2) [\text{Re}(Z_6 Z_7^*) - |Z_6|^2]\} \\
& + 2\text{Im}(Z_5^* Z_6^2 Z_7^2) \text{Re}(Z_5^* Z_6^2 Z_7^2) - 2\text{Im}(Z_5^* Z_6^2 Z_7^2) \text{Re}(Z_5^* Z_6 Z_7) - 2\text{Re}(Z_5^* Z_6^2 Z_7^2) \text{Im}(Z_5^* Z_6 Z_7) \\
& - (Z_1 - Z_2) (Z_1 - Z_{34})^2 \text{Im}(Z_5^* Z_6^2 Z_7^2) + (Z_1 - Z_2)^2 (Z_1 + Z_2 - 2Z_{34}) \text{Im}(Z_5^* Z_6 Z_7) \\
& + 2(Z_1 - Z_2) [\text{Re}(Z_6 Z_7^*) \text{Im}(Z_5^* Z_6^2 Z_7^2) - f_1 \text{Im}(Z_5^* Z_6 Z_7)] + (Z_1 - Z_2)^3 \text{Im}(Z_5^* Z_6 Z_7), \tag{172}
\end{aligned}$$

where the f_i are defined in Eq. (95).

Case 4.— $\text{Im}(m_{12}^2 \lambda_6^*) = 0$, $m_{12}^2 \neq 0$ and $\lambda_1 \neq \lambda_2$.

In this case, Eqs. (162)–(165) yield $I_{Y3Z} = 0$ and

$$I_{2Y2Z} = (\lambda_1 - \lambda_2) \text{Im}(\lambda_5^* [m_{12}^2]^2), \tag{173}$$

$$I_{6Z} = - \left(\frac{(\lambda_1 - \lambda_2)^2 \text{Re}[(m_{12}^2 \lambda_6^*)^2]}{|m_{12}^2|^4} \right) I_{2Y2Z}. \tag{174}$$

As in the case of I_{6Z} , one sees that I_{3Y3Z} is also proportional to $\text{Im}(\lambda_5^* [m_{12}^2]^2)$. Both results can be understood geometrically by noting that the condition $\text{Im}(m_{12}^2 \lambda_6^*) = 0$ implies that m_{12}^2 and λ_6 are aligned in the complex plane, whereas

$\text{Im}(\lambda_5^* [m_{12}^2]^2) = 0$ implies that $[m_{12}^2]^2$ and λ_5 are aligned in the complex plane. Hence, if $I_{2Y2Z} = 0$, then $[m_{12}^2]^2 \lambda_6$ and λ_6^2 are aligned with λ_5 , and it follows that $I_{6Z} = 0$ and $I_{3Y3Z} = 0$. Once again, only one invariant quantity, I_{2Y2Z} , is needed to determine whether the scalar potential is explicitly CP conserving.

To be complete, we examine two further cases in which $I_{Y3Z} \neq 0$, where only one CP-odd invariant is needed to determine whether the scalar potential is explicitly CP conserving.

Case 5.— $\text{Im}(\lambda_5^* [m_{12}^2]^2) = (m_{11}^2 - m_{22}^2) \text{Im}(m_{12}^2 \lambda_6^*)$, $m_{12}^2 \neq 0$ and $\lambda_1 \neq \lambda_2$.

In this case, Eqs. (162)–(165) yield $I_{2Y2Z} = 0$ and

$$I_{Y3Z} = (\lambda_1 - \lambda_2)^2 \text{Im}(m_{12}^2 \lambda_6^*), \tag{175}$$

$$I_{6Z} = \left(\frac{(\lambda_1 - \lambda_2) [2\text{Re}(m_{12}^2 \lambda_6^*) \text{Re}(\lambda_5^* [m_{12}^2]^2) - (m_{11}^2 - m_{22}^2) \text{Re}[(m_{12}^2 \lambda_6^*)^2]]}{|m_{12}^2|^4} \right) I_{Y3Z}. \tag{176}$$

One can show that I_{3Y3Z} is also proportional to $\text{Im}(m_{12}^2 \lambda_6^*)$. Hence, if $I_{Y3Z} = 0$, then it follows that $I_{6Z} = I_{3Y3Z} = 0$. That is, only one invariant quantity, I_{Y3Z} , is needed to determine whether the scalar potential is explicitly CP conserving.

Case 6.— $\lambda_5 = 0$ and $\lambda_1 \neq \lambda_2$.

In this case, Eqs. (162)–(165) yield $I_{6Z} = 0$ and

$$I_{Y3Z} = (\lambda_1 - \lambda_2)^2 \text{Im}(m_{12}^2 \lambda_6^*), \tag{177}$$

$$I_{2Y2Z} = - \left(\frac{m_{11}^2 - m_{22}^2}{\lambda_1 - \lambda_2} \right) I_{Y3Z}. \tag{178}$$

As in the previous case, one can show that I_{3Y3Z} is also proportional to $\text{Im}(m_{12}^2 \lambda_6^*)$. Hence, if $I_{Y3Z} = 0$, then it follows that $I_{2Y2Z} = I_{3Y3Z} = 0$. That is, only one invariant quantity, I_{Y3Z} , is needed to determine whether the scalar potential is explicitly CP conserving.

In summary, in generic regions of the 2HDM parameter space, it is sufficient to examine two CP-odd invariant quantities, I_{Y3Z} and I_{2Y2Z} given in Eqs. (156) and (157) in order to determine whether or not the scalar potential

explicitly breaks the CP symmetry. In special regions of parameter space examined in the six cases above, one CP-odd invariant quantity is sufficient, although in some cases a third CP-odd invariant, I_{6Z} , or a fourth CP-odd invariant, I_{3Y3Z} , is needed to determine the CP property of the scalar potential. In the Lee model of spontaneous CP violation, all four CP-odd invariants vanish, and the scalar potential is explicitly CP conserving, but at least one of the invariants, $\text{Im}(Z_6^2 Z_5^*)$, $\text{Im}(Z_7^2 Z_5^*)$, and $\text{Im}(Z_6 Z_7^*)$ is nonvanishing, signaling that in the absence of explicit CP violation, the source of the CP violation must be attributed to the properties of the vacuum.

VIII. CONCLUSIONS

The C2HDM is the most general two-Higgs-doublet model that possesses a softly broken \mathbb{Z}_2 symmetry (the latter is imposed to eliminate tree-level Higgs-mediated FCNCs). In the so-called \mathbb{Z}_2 basis where the \mathbb{Z}_2 symmetry of the quartic terms in the scalar potential is manifestly realized, one can rephase the scalar fields such that the vevs v_1 and v_2 are real and non-negative. After minimizing the scalar potential and fixing $v = (v_1^2 + v_2^2)^{1/2} = 246$ GeV,

the C2HDM is governed by nine additional real parameters: four scalar masses, one additional squared-mass parameter, $\text{Re } m_{12}^2$, $\tan \beta = v_2/v_1$, and three mixing angles arising from the diagonalization of the neutral scalar squared-mass matrix. One sum rule [cf. Eq. (147)] reduces the total number of independent degrees of freedom (including v) to nine.

In this paper, we have provided a basis-invariant treatment of the C2HDM. This involves a number of steps. First, we transformed to the Higgs basis, which is defined up to an arbitrary rephasing of the Higgs basis field H_2 (which by definition possesses no vacuum expectation value). Consequently, the real parameters of the Higgs basis scalar potential are invariant quantities, whereas the complex parameters are pseudoinvariant quantities that are rephased under $H_2 \rightarrow e^{i\chi} H_2$. This allows us to easily identify basis-independent quantities, which are related to physical observables of the model. The softly broken \mathbb{Z}_2 symmetry constrains the Higgs basis parameters and yields one complex invariant constraint equation. Our results are consistent with the more formal results of Ref. [33] and a recent computation of Ref. [58] that was carried out in a convention of real vevs in the \mathbb{Z}_2 basis. For completeness, we have also provided the corresponding constraints if the \mathbb{Z}_2 symmetry is extended to incorporate the dimension-two squared-mass terms of the scalar potential.

Having obtained the constraints due to the presence of a softly broken \mathbb{Z}_2 symmetry, one can check that the C2HDM is governed by nine basis-independent parameters in agreement with our previous counting above. Moreover, one can now identify the behavior of the parameters of the C2HDM under basis transformations. Our analysis revealed that some combinations of the mixing angles α_1 , α_2 , and α_3 and the parameter $\tan \beta$ possess a residual basis dependence due to the freedom to interchange the two complex scalar doublet fields of the C2HDM. In practice, this residual basis dependence is removed by declaring that $\tan \beta < 1$ corresponds to an enhanced coupling of some of the neutral Higgs bosons to up-type quarks. Having adopted this convention (which is implicitly assumed in the literature but never stated explicitly), the angle parameters of the C2HDM and the parameter $\tan \beta$ are promoted to basis-independent quantities that can be directly related to physical observables.

Our work also resolves an apparent conflict between the number of physical phases in the matrices that diagonalize the squared-mass matrix of the neutral Higgs fields that arise in the two approaches. Indeed, the basis-invariant calculation exhibited in Sec. III involves two basis-invariant angles (θ_{12} and θ_{13}), and one unphysical angle (θ_{23}), whereas the calculations in the C2HDM resulting in Eq. (141) yields three physical angles $\alpha_{1,2,3}$. The resolution of this conundrum is associated with the observation that the C2HDM is initially defined in a \mathbb{Z}_2 basis where both vevs are real. The constraint imposed by the reality of the

two vevs ultimately allows one to ascribe physical significance to the pseudoinvariant quantity, θ_{23} . This can be seen directly in Eq. (77) which relates the relative phase of the two vevs to the phase of the pseudoinvariant quantity Z_{67} . Thus, by fixing the phase of the two vevs to be zero, one fixes the quantity Z_{67} to be real. This leaves a sign ambiguity that is resolved once a twofold ambiguity in the definition of $\tan \beta$ is fixed as indicated above. We have also examined special cases in which $Z_{67} = 0$, where the phase of Z_6 is similarly fixed in the convention of real vevs.¹⁵ The so-called exceptional region of the 2HDM parameter space where $Z_1 = Z_2$ and $Z_{67} = 0$ requires special attention and is treated in Appendix B.

Finally, we have reanalyzed the techniques for detecting the presence of discrete symmetries originally presented by Lavoura in Ref. [46]. We have obtained results that are in agreement with the corresponding results in Lavoura's paper (after correcting one typographical error in Ref. [46]). In addition, we have extended Lavoura's results in two directions. First, we noted that the invariant constraints obtained by Lavoura do not apply in all parameter regimes of the C2HDM. Some special cases require additional analysis, and we have provided the appropriate modifications in cases that cannot be obtained directly from considerations of the generic regions of the parameter space. Second, Lavoura was only able to obtain one of two relations that must be satisfied in the 2HDM with an explicitly CP-conserving scalar potential but with no (unbroken or broken) \mathbb{Z}_2 symmetry that exhibits spontaneous CP violation (i.e., the Lee model [1]). We have provided the second relation that was missed by Lavoura (using the results obtained in Ref. [59]), and we have clarified a number of special cases in which only one relation is sufficient (although that relation is typically not the one found by Lavoura). It is also instructive to apply this analysis in the presence of a softly broken \mathbb{Z}_2 symmetry. In doing so, we noted a surprising aspect of a subset of the exceptional region of the parameter space where no \mathbb{Z}_2 basis exists where all the scalar potential parameters are real, and yet the corresponding 2HDM is CP conserving.

In conclusion, the basis-independent formalism possesses many advantages. For example, just like covariance in relativistic theories where an equation can be checked by ensuring that both sides of the equation behave similarly under Lorentz transformations in the same way, the basis-independent formalism affords similar benefits. Indeed, errors in numerous equations in this paper were avoided by such considerations. In addition, due to the close connection of basis-independent quantities to physical observables, one obtains confidence in appreciating the significance of the relations among the various 2HDM parametrizations.

¹⁵If $Z_6 = Z_7 = 0$, then the model reduces to the IDM discussed in Sec. VA. This model is necessarily CP conserving and thus is not of further interest to us in this work.

We hope that the application of basis-independent methods in the analysis of the C2HDM presented in this paper has contributed to a better understanding of this model and will be useful in future phenomenological studies of CP-violating Higgs phenomena.

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APPENDIX A: CHANGING THE BASIS OF SCALAR FIELDS IN THE 2HDM

Since the scalar doublets Φ_1 and Φ_2 have identical $SU(2) \times U(1)$ quantum numbers, one is free to define two orthonormal linear combinations of the original scalar fields. The parameters appearing in Eq. (2) 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 $\Phi' = U\Phi$, where U is a $U(2)$ matrix,

$$U = \begin{pmatrix} \cos \beta & e^{-i\xi} \sin \beta \\ -e^{i(\xi+\eta)} \sin \beta & e^{i\eta} \cos \beta \end{pmatrix}, \quad (\text{A1})$$

up to an overall complex phase factor $e^{i\psi}$ that has no effect on the scalar potential parameters, since this corresponds to a global hypercharge transformation.

With respect to the new Φ' basis, the scalar potential takes on the same form given in Eq. (2) but with new coefficients m'_{ij} and λ'_j . For the general $U(2)$ transformation of Eq. (A1) with $\Phi' = U\Phi$, the scalar potential parameters (m'_{ij}, λ'_j) are related to the original parameters (m_{ij}^2, λ_i) by

$$m'^2_{11} = m^2_{11} c_\beta^2 + m^2_{22} s_\beta^2 - \text{Re}(m^2_{12} e^{i\xi}) s_{2\beta}, \quad (\text{A2})$$

$$m'^2_{22} = m^2_{11} s_\beta^2 + m^2_{22} c_\beta^2 + \text{Re}(m^2_{12} e^{i\xi}) s_{2\beta}, \quad (\text{A3})$$

$$m'^2_{12} e^{i(\xi+\eta)} = \frac{1}{2}(m^2_{11} - m^2_{22}) s_{2\beta} + \text{Re}(m^2_{12} e^{i\xi}) c_{2\beta} + i \text{Im}(m^2_{12} e^{i\xi}), \quad (\text{A4})$$

$$\lambda'_1 = \lambda_1 c_\beta^4 + \lambda_2 s_\beta^4 + \frac{1}{2} \lambda_{345} s_{2\beta}^2 + 2s_{2\beta} [c_\beta^2 \text{Re}(\lambda_6 e^{i\xi}) + s_\beta^2 \text{Re}(\lambda_7 e^{i\xi})], \quad (\text{A5})$$

$$\lambda'_2 = \lambda_1 s_\beta^4 + \lambda_2 c_\beta^4 + \frac{1}{2} \lambda_{345} s_{2\beta}^2 - 2s_{2\beta} [s_\beta^2 \text{Re}(\lambda_6 e^{i\xi}) + c_\beta^2 \text{Re}(\lambda_7 e^{i\xi})], \quad (\text{A6})$$

$$\lambda'_3 = \frac{1}{4} s_{2\beta}^2 [\lambda_1 + \lambda_2 - 2\lambda_{345}] + \lambda_3 - s_{2\beta} c_{2\beta} \text{Re}[(\lambda_6 - \lambda_7) e^{i\xi}], \quad (\text{A7})$$

$$\lambda'_4 = \frac{1}{4} s_{2\beta}^2 [\lambda_1 + \lambda_2 - 2\lambda_{345}] + \lambda_4 - s_{2\beta} c_{2\beta} \text{Re}[(\lambda_6 - \lambda_7) e^{i\xi}], \quad (\text{A8})$$

$$\begin{aligned} \lambda'_5 e^{2i(\xi+\eta)} &= \frac{1}{4} s_{2\beta}^2 [\lambda_1 + \lambda_2 - 2\lambda_{345}] + \text{Re}(\lambda_5 e^{2i\xi}) + i c_{2\beta} \text{Im}(\lambda_5 e^{2i\xi}) - s_{2\beta} c_{2\beta} \text{Re}[(\lambda_6 - \lambda_7) e^{i\xi}] \\ &\quad - i s_{2\beta} \text{Im}[(\lambda_6 - \lambda_7) e^{i\xi}], \end{aligned} \quad (\text{A9})$$

$$\begin{aligned} \lambda'_6 e^{i(\xi+\eta)} &= -\frac{1}{2} s_{2\beta} [\lambda_1 c_\beta^2 - \lambda_2 s_\beta^2 - \lambda_{345} c_{2\beta} - i \text{Im}(\lambda_5 e^{2i\xi})] + c_\beta c_{3\beta} \text{Re}(\lambda_6 e^{i\xi}) + s_\beta s_{3\beta} \text{Re}(\lambda_7 e^{i\xi}) \\ &\quad + i c_\beta^2 \text{Im}(\lambda_6 e^{i\xi}) + i s_\beta^2 \text{Im}(\lambda_7 e^{i\xi}), \end{aligned} \quad (\text{A10})$$

$$\begin{aligned} \lambda'_7 e^{i(\xi+\eta)} &= -\frac{1}{2} s_{2\beta} [\lambda_1 s_\beta^2 - \lambda_2 c_\beta^2 + \lambda_{345} c_{2\beta} + i \text{Im}(\lambda_5 e^{2i\xi})] + s_\beta s_{3\beta} \text{Re}(\lambda_6 e^{i\xi}) + c_\beta c_{3\beta} \text{Re}(\lambda_7 e^{i\xi}) \\ &\quad + i s_\beta^2 \text{Im}(\lambda_6 e^{i\xi}) + i c_\beta^2 \text{Im}(\lambda_7 e^{i\xi}), \end{aligned} \quad (\text{A11})$$

where $s_\beta \equiv \sin \beta$, $c_\beta \equiv \cos \beta$, etc., and

$$\lambda_{345} \equiv \lambda_3 + \lambda_4 + \text{Re}(\lambda_5 e^{2i\xi}). \quad (\text{A12})$$

We shall make use of Eqs. (A2)–(A11) to write out the explicit relations between the scalar potential parameters of a generic basis and the Higgs basis. We can employ the unitary matrix given by Eq. (A1), where

$$\tan \beta \equiv \frac{v_2}{v_1}, \quad (\text{A13})$$

and v_1 and v_2 are the magnitudes of the vevs of the neutral components of the Higgs fields in the generic basis, defined in Eq. (3). In particular,

$$v_1 = v \cos \beta, \quad v_2 = v \sin \beta \quad (\text{A14})$$

are non-negative quantities, which implies that we may assume that $0 \leq \beta \leq \frac{1}{2}\pi$. It follows that the invariant Higgs basis fields defined in Eq. (25) are given by

$$\begin{pmatrix} \mathcal{H}_1 \\ \mathcal{H}_2 \end{pmatrix} = \begin{pmatrix} \cos \beta & e^{-i\xi} \sin \beta \\ -e^{i(\xi+\eta)} \sin \beta & e^{i\eta} \cos \beta \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}. \quad (\text{A15})$$

Consequently, we can identify the primed scalar potential parameters with the scalar potential coefficients of the Higgs basis, $\{\mathcal{H}_1, \mathcal{H}_2\}$, as specified in Eq. (28).

As an example, if the Φ' basis is identified with the Higgs basis then, e.g., $\lambda'_1 = Z_1$, $\lambda'_2 = Z_2$, $\lambda'_6 = Z_6 e^{-i\eta}$, $\lambda'_7 = Z_7 e^{-i\eta}$, etc. In particular, the η dependence on the

left-hand side of Eqs. (A4) and (A9)–(A11) cancels out. Hence, if we identify the Φ basis as a \mathbb{Z}_2 basis where $\lambda_6 = \lambda_7 = 0$, it then follows from Eqs. (A5), (A6), (A10), and (A11) that

$$Z_1 - Z_2 = (\lambda_1 - \lambda_2)c_{2\beta}, \quad Z_{67}e^{i\xi} = -\frac{1}{2}s_{2\beta}(\lambda_1 - \lambda_2). \quad (\text{A16})$$

Consequently,

$$\frac{1}{2}(Z_1 - Z_2)s_{2\beta} + c_{2\beta}Z_{67}e^{i\xi} = 0. \quad (\text{A17})$$

Noting that Eq. (A16) implies that $\text{Im}(Z_{67}e^{i\xi}) = 0$; it follows that Eqs. (70) and (A17) are consistent equations.

It is convenient to invert the resulting equations and express the m_{ij}^2 and λ_i in terms of the Y_i and Z_i . This is easily done by employing the inverse matrix $U^{-1} = U^\dagger$, which simply corresponds to taking $\beta \rightarrow -\beta$, $\eta \rightarrow -\eta$ and $\xi \rightarrow \xi + \eta$ (the last two replacements are equivalent to the interchange of $\xi \leftrightarrow \xi + \eta$). Hence, it follows that¹⁶

$$m_{11}^2 = Y_1 c_\beta^2 + Y_2 s_\beta^2 - \text{Re}(Y_3 e^{i\xi})s_{2\beta}, \quad (\text{A18})$$

$$m_{22}^2 = Y_1 s_\beta^2 + Y_2 c_\beta^2 + \text{Re}(Y_3 e^{i\xi})s_{2\beta}, \quad (\text{A19})$$

$$m_{12}^2 e^{i\xi} = \frac{1}{2}(Y_2 - Y_1)s_{2\beta} - \text{Re}(Y_3 e^{i\xi})c_{2\beta} - i\text{Im}(Y_3 e^{i\xi}) \quad (\text{A20})$$

and

$$\lambda_1 = Z_1 c_\beta^4 + Z_2 s_\beta^4 + \frac{1}{2}Z_{345}s_{2\beta}^2 - 2s_{2\beta}[c_\beta^2 \text{Re}(Z_6 e^{i\xi}) + s_\beta^2 \text{Re}(Z_7 e^{i\xi})], \quad (\text{A21})$$

$$\lambda_2 = Z_1 s_\beta^4 + Z_2 c_\beta^4 + \frac{1}{2}Z_{345}s_{2\beta}^2 + 2s_{2\beta}[s_\beta^2 \text{Re}(Z_6 e^{i\xi}) + c_\beta^2 \text{Re}(Z_7 e^{i\xi})], \quad (\text{A22})$$

$$\lambda_3 = \frac{1}{4}s_{2\beta}^2[Z_1 + Z_2 - 2Z_{345}] + Z_3 + s_{2\beta}c_{2\beta} \text{Re}[(Z_6 - Z_7)e^{i\xi}], \quad (\text{A23})$$

$$\lambda_4 = \frac{1}{4}s_{2\beta}^2[Z_1 + Z_2 - 2Z_{345}] + Z_4 + s_{2\beta}c_{2\beta} \text{Re}[(Z_6 - Z_7)e^{i\xi}], \quad (\text{A24})$$

$$\begin{aligned} \lambda_5 e^{2i\xi} &= \frac{1}{4}s_{2\beta}^2[Z_1 + Z_2 - 2Z_{345}] + \text{Re}(Z_5 e^{2i\xi}) + ic_{2\beta} \text{Im}(Z_5 e^{2i\xi}) \\ &\quad + s_{2\beta}c_{2\beta} \text{Re}[(Z_6 - Z_7)e^{i\xi}] + is_{2\beta} \text{Im}[(Z_6 - Z_7)e^{i\xi}], \end{aligned} \quad (\text{A25})$$

$$\begin{aligned} \lambda_6 e^{i\xi} &= \frac{1}{2}s_{2\beta}[Z_1 c_\beta^2 - Z_2 s_\beta^2 - Z_{345}c_{2\beta} - i\text{Im}(Z_5 e^{2i\xi})] + c_\beta c_{3\beta} \text{Re}(Z_6 e^{i\xi}) \\ &\quad + s_\beta s_{3\beta} \text{Re}(Z_7 e^{i\xi}) + ic_\beta^2 \text{Im}(Z_6 e^{i\xi}) + is_\beta^2 \text{Im}(Z_7 e^{i\xi}), \end{aligned} \quad (\text{A26})$$

¹⁶Note that the sign in front of Y_3 in Eq. (28) is positive, whereas the sign in front of m_{12}^2 in Eq. (2) is negative. Thus, we have identified $Y_3 = -m_{12}^2$ in obtaining Eqs. (A18)–(A20) from Eqs. (A2)–(A4).

$$\begin{aligned} \lambda_7 e^{i\xi} = & \frac{1}{2} s_{2\beta} [Z_1 s_\beta^2 - Z_2 c_\beta^2 + Z_{345} c_{2\beta} + i \text{Im}(Z_5 e^{2i\xi})] + s_\beta s_{3\beta} \text{Re}(Z_6 e^{i\xi}) \\ & + c_\beta c_{3\beta} \text{Re}(Z_7 e^{i\xi}) + i s_\beta^2 \text{Im}(Z_6 e^{i\xi}) + i c_\beta^2 \text{Im}(Z_7 e^{i\xi}), \end{aligned} \quad (\text{A27})$$

where

$$Z_{345} \equiv Z_3 + Z_4 + \text{Re}(Z_5 e^{2i\xi}). \quad (\text{A28})$$

It is convenient to take the sum and difference of Eqs. (A26) and (A27) to obtain

$$(\lambda_6 + \lambda_7) e^{i\xi} = \frac{1}{2} s_{2\beta} (Z_1 - Z_2) + c_{2\beta} \text{Re}[(Z_6 + Z_7) e^{i\xi}] + i \text{Im}[(Z_6 + Z_7) e^{i\xi}], \quad (\text{A29})$$

$$(\lambda_6 - \lambda_7) e^{i\xi} = \frac{1}{2} s_{2\beta} c_{2\beta} (Z_1 + Z_2 - 2Z_{345}) - i s_{2\beta} \text{Im}(Z_5 e^{2i\xi}) + c_{4\beta} \text{Re}[(Z_6 - Z_7) e^{i\xi}] + i c_{2\beta} \text{Im}[(Z_6 - Z_7) e^{i\xi}]. \quad (\text{A30})$$

As previously noted, all factors of $e^{i\eta}$ have canceled out due to the η dependence of the coefficients of the Higgs basis scalar potential given in Eq. (28).

APPENDIX B: THE EXCEPTIONAL CASE OF $Z_1 = Z_2$ AND $Z_7 = -Z_6$

In the exceptional case of $Z_1 = Z_2$ and $Z_7 = -Z_6$, it follows from Eqs. (A21)–(A27) that $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ in all scalar field bases.¹⁷ In this appendix, we show that in this exceptional case, there exists a Φ basis in which $\lambda_6 = \lambda_7 = 0$. That is, there exists a scalar field basis where the \mathbb{Z}_2 symmetry of the quartic terms of the scalar potential is manifest.

It we set $Z_1 = Z_2$ and $Z_{67} = 0$ in Eqs. (A26) and (A27), then it follows that a scalar basis with $\lambda_6 = \lambda_7 = 0$ exists if and only if values of β and ξ can be found such that

$$\begin{aligned} s_{2\beta} c_{2\beta} [Z_1 - Z_{34} - \text{Re}(Z_5 e^{2i\xi})] - i s_{2\beta} \text{Im}(Z_5 e^{2i\xi}) \\ + 2c_{4\beta} \text{Re}(Z_6 e^{i\xi}) + 2i c_{2\beta} \text{Im}(Z_6 e^{i\xi}) = 0. \end{aligned} \quad (\text{B1})$$

Taking the real and imaginary parts of Eq. (B1) yields

$$s_{2\beta} \text{Im}(Z_5 e^{2i\xi}) = 2c_{2\beta} \text{Im}(Z_6 e^{i\xi}), \quad (\text{B2})$$

¹⁷We note in passing that the exceptional region of parameter space where $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$ was identified in Ref. [47] as the conditions for a softly broken CP2-symmetric scalar potential, where CP2 is the generalized CP transformation, $\Phi_1 \rightarrow \Phi_2^*$ and $\Phi_2 \rightarrow -\Phi_1^*$. In general, dimension-two soft CP2-breaking squared-mass terms are present and violate the CP2-symmetric conditions, $m_{11}^2 = m_{22}^2$ and $m_{12}^2 = 0$. However, the CP2 symmetry is also violated by the dimension-four Yukawa interactions, which constitute a hard breaking of the symmetry [64]. Consequently, the exceptional region of the parameter space is unnatural and must be regarded as finely tuned.

$$s_{2\beta} c_{2\beta} [Z_1 - Z_{34} - \text{Re}(Z_5 e^{2i\xi})] = -2c_{4\beta} \text{Re}(Z_6 e^{i\xi}). \quad (\text{B3})$$

If there exists a scalar basis in which $\lambda_6 = \lambda_7 = 0$, then this basis is not unique since the relation $\lambda_6 = \lambda_7 = 0$ is unchanged under the basis transformation, $\Phi_a \rightarrow U_{ab} \Phi_b$, where U is given by Eq. (72). Indeed, Eqs. (B2) and (B3) are unchanged under the transformations exhibited in Eq. (74), as expected. Thus, when solving Eqs. (B2) and (B3), we expect at least a twofold ambiguity in the determination of β and ξ (where $0 \leq \beta \leq \frac{1}{2}\pi$ and $0 \leq \xi < 2\pi$).

If $Z_6 = 0$, then the scalar potential in the Higgs basis manifestly exhibits the \mathbb{Z}_2 symmetry, so we shall henceforth assume that $Z_6 \neq 0$, in which case we may write $Z_6 \equiv |Z_6| e^{i\theta_6}$. It is convenient to introduce

$$\xi' \equiv \xi + \theta_6. \quad (\text{B4})$$

Under the basis transformation $\Phi_a \rightarrow U_{ab} \Phi_b$, where U is given by Eq. (72), it follows that $e^{i\xi'} \rightarrow -e^{i\xi'}$, in light of Eq. (74). That is, ξ' is only determined modulo π , corresponding to the twofold ambiguity anticipated above.

Inserting $e^{i\xi} = e^{i\xi'} Z_6^* / |Z_6|$ into Eqs. (B2) and (B3) yields

$$s_{2\beta} [\text{Re}(Z_5^* Z_6^2) \sin 2\xi' - \text{Im}(Z_5^* Z_6^2) \cos 2\xi'] = 2c_{2\beta} |Z_6|^3 \sin \xi', \quad (\text{B5})$$

$$\begin{aligned} s_{2\beta} c_{2\beta} [|Z_6|^2 (Z_1 - Z_{34}) - \text{Re}(Z_5^* Z_6^2) \cos 2\xi' \\ - \text{Im}(Z_5^* Z_6^2) \sin 2\xi'] = -2c_{4\beta} |Z_6|^3 \cos \xi'. \end{aligned} \quad (\text{B6})$$

We now consider two cases. First, if we assume that $\text{Im}(Z_5^* Z_6^2) = 0$ then $\sin \xi' = 0$ is a solution to Eq. (B5), which implies that $\cos \xi' = \pm 1$; the twofold ambiguity was anticipated in light of the comment following Eq. (B4).

Inserting $\cos \xi' = \pm 1$ into Eq. (B6) then yields a quadratic equation for $\cot 2\beta = c_{2\beta}/s_{2\beta}$,

$$2|Z_6|\cot^2 2\beta \pm \left(Z_1 - Z_{34} - \frac{\text{Re}(Z_5^* Z_6^2)}{|Z_6|^2} \right) \cot 2\beta - 2|Z_6| = 0. \quad (\text{B7})$$

As expected from Eq. (74), changing the sign of $\cos \xi'$ from +1 to -1 simply changes the sign of $\cot 2\beta$. Moreover, Eq. (B7) possesses two real roots whose product is equal to -1. This observation implies that if β is one solution of Eq. (B7), then the second solution is $\beta \pm \frac{1}{4}\pi$ (where the sign is chosen such that the second solution lies between 0 and $\frac{1}{2}\pi$). Hence, if $Z_1 = Z_2$, $Z_{67} = 0$, and $\text{Im}(Z_5^* Z_6^2) = 0$, then there are four choices of (β, ξ) , where $0 \leq \beta \leq \frac{1}{2}\pi$ and $\cos \xi' = \pm 1$, in which Eqs. (B2) and (B3) are satisfied.

If $\text{Im}(Z_5^* Z_6^2) = 0$ and $\sin \xi' \neq 0$, then additional solutions of Eqs. (B5) and (B6) exist. Solving Eq. (B5) for $c_{2\beta}/s_{2\beta}$ and inserting this result into Eq. (B6) yield

$$\cos \xi' \{ [\text{Re}(Z_5^* Z_6^2)]^2 + \text{Re}(Z_5^* Z_6^2) |Z_6|^2 (Z_1 - Z_{34}) - 2|Z_6|^6 \} = 0. \quad (\text{B8})$$

Since the coefficient of $\cos \xi'$ is generically nonzero, it follows that $\cos \xi' = 0$. Plugging this result back into Eq. (B5) yields $\cos 2\beta = 0$. Hence, $(\beta = \frac{1}{4}\pi, \xi' = \frac{1}{2}\pi)$ and $(\beta = \frac{3}{4}\pi, \xi' = \frac{3}{2}\pi)$ are also solutions to Eqs. (B5) and (B6) when $\text{Im}(Z_5^* Z_6^2) = 0$. These two solutions are again related by the basis transformation $\Phi_a \rightarrow U_{a\bar{b}} \Phi_b$, where U is given by Eq. (72).

Second, if we assume instead that $\text{Im}(Z_5^* Z_6^2) \neq 0$, then $\sin \xi' \neq 0$. In this case, we follow the method employed in Appendix C of Ref. [59]. Solving Eq. (B5) for $s_{2\beta}/c_{2\beta}$ and

inserting this result into Eq. (B6) yield the following equation for ξ' :

$$F(\xi') \equiv \sin \xi' [R \sin 2\xi' - I \cos 2\xi'] \times [|Z_6|^2 (Z_1 - Z_{34}) - R \cos 2\xi' - I \sin 2\xi'] + \cos \xi' [(R \sin 2\xi' - I \cos 2\xi')^2 - 4|Z_6|^6 \sin^2 \xi'] = 0, \quad (\text{B9})$$

where $R \equiv \text{Re}(Z_5^* Z_6^2)$ and $I \equiv \text{Im}(Z_5^* Z_6^2)$. Noting that $F(\xi' + \pi) = -F(\xi')$, it follows that Eq. (B9) determines ξ' modulo π , as expected in light of the comment below [Eq. (B4)]. Moreover, given that $F(\xi' = 0) = I^2$ and $F(\xi' = \pi) = -I^2$, there must exist an angle ξ'_0 such that $0 < \xi'_0 < \pi$ and $F(\xi'_0) = 0$. Plugging $\xi' = \xi'_0$ back into Eq. (B5) then yields

$$\cot 2\beta = \frac{R \sin 2\xi'_0 - I \cos 2\xi'_0}{2|Z_6|^3 \sin \xi'_0}. \quad (\text{B10})$$

As expected, under a basis transformation, $\Phi_a \rightarrow U_{a\bar{b}} \Phi_b$, where U is given by Eq. (72), it follows that $\xi'_0 \rightarrow \xi'_0 + \pi$ and $\cot 2\beta \rightarrow -\cot 2\beta$, which is consistent with Eq. (B10).

Thus, we have shown that there are at least two choices of (β, ξ) , where $0 \leq \beta \leq \frac{1}{2}\pi$ and $0 \leq \xi < 2\pi$, that satisfy Eq. (B1). That is, we have proven that if $Z_1 = Z_2$ and $Z_{67} = 0$, then a scalar basis exists in which $\lambda_6 = \lambda_7 = 0$, where the softly broken \mathbb{Z}_2 symmetry is manifestly realized.

We end this appendix with a discussion of spontaneous CP violation. Starting from Eq. (94), we can eliminate $\text{Re}(Z_5 e^{2i\xi})$ and $\text{Im}(Z_5 e^{2i\xi})$ by employing Eqs. (B2) and (B3). If we denote $\mathcal{R} \equiv \text{Re}(Z_6 e^{i\xi}) = |Z_6| \cos \xi'$ and $\mathcal{I} \equiv \text{Im}(Z_6 e^{i\xi}) = |Z_6| \sin \xi'$, the end result is

$$\text{Im}(\lambda_5^* [m_{12}^2]^2) = -\frac{v^4}{8c_{2\beta}s_{2\beta}} \mathcal{I} \left\{ 4c_{2\beta}s_{2\beta}^2 \left(\frac{Y_2}{v^2} \right)^2 + 4s_{2\beta}^2 \left(\frac{Y_2}{v^2} \right) [s_{2\beta}\mathcal{R} + c_{2\beta}Z_{34}] - 4c_{2\beta}\mathcal{I}^2 - 4c_{2\beta}c_{4\beta}\mathcal{R}^2 - 2s_{2\beta}[c_{4\beta}Z_1 + c_{2\beta}^2(Z_1 - 2Z_{34})]\mathcal{R} - c_{2\beta}s_{2\beta}^2 Z_1(Z_1 - 2Z_{34}) \right\}, \quad (\text{B11})$$

where λ_5 and m_{12}^2 are parameters of the scalar potential in the \mathbb{Z}_2 basis, and β and ξ are solutions to Eqs. (B2) and (B3).

Below Eq. (B6), we showed that if $\text{Im}(Z_5^* Z_6^2) = 0$, then one solution to Eqs. (B2) and (B3) is $\sin \xi' = 0$. In this case, $\mathcal{I} = \text{Im}(Z_6 e^{i\xi}) = |Z_6| \sin \xi' = 0$, and it immediately follows from Eq. (B11) that $\text{Im}(\lambda_5^* [m_{12}^2]^2) = 0$. We also showed above that if $\text{Im}(Z_5^* Z_6^2) = 0$, then a second solution exists in which $c_{2\beta} = 0$ and $\cos \xi' = 0$. In order to employ Eq. (B11) in this case, one must first use Eq. (B3) in order to rewrite $\text{Im}(\lambda_5^* [m_{12}^2]^2)$ in terms of \mathcal{I} and $\text{Re}(Z_5 e^{2i\xi})$. Having done so, the factor of $c_{2\beta}$ in the denominator

of the prefactor in Eq. (B11) cancels out, and one can then set $c_{2\beta} = 0$. Finally, we employ $\text{Re}(Z_5 e^{2i\xi}) = -\text{Re}(Z_5^* Z_6^2)/|Z_6|^2$ (after using $e^{2i\xi} = e^{2i\xi'} (Z_6^*)^2/|Z_6|^2$ and $\cos 2\xi' = -1$). The resulting expression reproduces Eq. (109) and yields $\text{Im}(\lambda_5^* [m_{12}^2]^2) \neq 0$, which implies that no \mathbb{Z}_2 basis exists in which m_{12}^2 and λ_5 are both real. Nevertheless, because $\text{Im}(Z_5^* Z_6^2) = 0$ and $Z_{67} = 0$, it follows that a real Higgs basis exists, which signifies that the scalar sector is CP conserving.

If $\text{Im}(Z_5^* Z_6^2) \neq 0$, then no real Higgs basis exists, and thus the scalar sector violates CP either explicitly or spontaneously. In this case, $\sin \xi' = \sin \xi'_0 \neq 0$, where

ξ'_0 is determined as discussed below Eq. (B9). Since CP is explicitly conserved if $\text{Im}(\lambda_5^*[m_{12}^2]^2) = 0$, it follows from Eq. (B11) that a basis-invariant condition for spontaneous CP violation is given by

$$4c_{2\beta}s_{2\beta}^2\left(\frac{Y_2}{v^2}\right)^2 + 4s_{2\beta}\left(\frac{Y_2}{v^2}\right)[s_{2\beta}\mathcal{R} + c_{2\beta}Z_{34}] - 4c_{2\beta}(\mathcal{I}^2 + c_{4\beta}\mathcal{R}^2) - 2s_{2\beta}[c_{4\beta}Z_1 + c_{2\beta}^2(Z_1 - 2Z_{34})]\mathcal{R} - c_{2\beta}s_{2\beta}^2Z_1(Z_1 - 2Z_{34}) = 0, \quad (\text{B12})$$

where $\mathcal{R} = |Z_6|\cos\xi'_0$ and $\mathcal{I} = |Z_6|\sin\xi'_0$, and the angle 2β is given by Eq. (B10).

APPENDIX C: BASIS-INVARIANT CONDITIONS FOR THE \mathbb{Z}_2 SYMMETRY REVISITED

In Sec. V, conditions for the presence of a \mathbb{Z}_2 symmetry in the scalar potential (which may or may not be softly broken) were derived. These conditions were expressed in terms of the Higgs basis scalar potential parameters and

were invariant with respect to an arbitrary rephasing of the Higgs basis field H_2 that defines the set of all possible Higgs bases. In Ref. [33], a set of manifestly basis-invariant expressions were presented which were sensitive to the presence of a \mathbb{Z}_2 symmetry in the 2HDM scalar potential.¹⁸ In this appendix, we demonstrate that if these expressions are evaluated in the Higgs basis, then the results of Sec. V are recovered.

We begin by defining two U(2)-flavor tensors constructed from the 2HDM couplings $Z_{\bar{a}b\bar{c}d}$ defined in Eq. (7),

$$Z_{\bar{a}d}^{(1)} \equiv \delta_{b\bar{c}}Z_{\bar{a}b\bar{c}d} = Z_{\bar{a}b\bar{b}d}, \quad Z_{\bar{c}d}^{(11)} \equiv Z_{\bar{b}a}^{(1)}Z_{\bar{a}b\bar{c}d}. \quad (\text{C1})$$

It is straightforward to work out the following explicit expressions in the Φ basis:

$$Z^{(1)} = \begin{pmatrix} \lambda_{14} & \lambda_{67} \\ \lambda_{67}^* & \lambda_{24} \end{pmatrix} \quad (\text{C2})$$

and

$$Z^{(11)} = \begin{pmatrix} \lambda_{14}\lambda_1 + \lambda_{24}\lambda_3 + \lambda_{67}\lambda_6^* + \lambda_{67}^*\lambda_6 & \lambda_{14}\lambda_6 + \lambda_{24}\lambda_7 + \lambda_{67}\lambda_4 + \lambda_{67}^*\lambda_5 \\ \lambda_{14}\lambda_6^* + \lambda_{24}\lambda_7^* + \lambda_{67}^*\lambda_4 + \lambda_{67}\lambda_5^* & \lambda_{14}\lambda_3 + \lambda_{24}\lambda_2 + \lambda_{67}\lambda_7^* + \lambda_{67}^*\lambda_7 \end{pmatrix}. \quad (\text{C3})$$

In Eqs. (C2) and (C3), we employ the shorthand notation, $\lambda_{ij} \equiv \lambda_i + \lambda_j$.

We now make use of the following result: starting from an arbitrary Φ basis of scalar fields, one can always transform to a Φ' basis in which $\lambda'_7 = -\lambda'_6$ [59]. A simple proof of this result is given in Appendix D. It is then straightforward to evaluate in the Φ' basis,

$$[Z^{(1)}, Z^{(11)}] = (\lambda'_1 - \lambda'_2)^2 \begin{pmatrix} 0 & \lambda'_6 \\ -\lambda'_6 & 0 \end{pmatrix}. \quad (\text{C4})$$

Assuming that $\lambda'_1 \neq \lambda'_2$ in a basis where $\lambda'_7 = -\lambda'_6$, it follows that if $[Z^{(1)}, Z^{(11)}] = 0$, then $\lambda'_6 = 0$. That is, in the Φ' basis, the softly broken \mathbb{Z}_2 symmetry is manifestly realized. In the special case of $\lambda'_1 = \lambda'_2$ and $\lambda'_7 = -\lambda'_6$, one can check from Eqs. (A5) to (A11) that $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$. That is, this condition holds in *all* scalar field bases. This result is not surprising given that in this special case, $Z_{\bar{a}b}^{(1)} = \lambda_{14}\delta_{\bar{a}b}$, which maintains this form under any U(2) transformation. Moreover, as shown in Appendix B, if $\lambda_1 = \lambda_2$ and $\lambda_7 = -\lambda_6$, then there exists scalar basis in which $\lambda_6 = \lambda_7 = 0$.

¹⁸The group theoretic analysis of the 2HDM scalar potential developed in Ref. [36] and the geometric picture of Ref. [40] provide alternative approaches for obtaining a basis-independent condition for the presence of a softly broken \mathbb{Z}_2 symmetry.

Hence, it follows that the condition for the existence of a softly broken \mathbb{Z}_2 symmetry that is manifest in some scalar field basis is given by [33]

$$[Z^{(1)}, Z^{(11)}] = 0. \quad (\text{C5})$$

Equation (C5) is covariant with respect to U(2) transformations. Hence, it can be evaluated in any scalar field basis. Thus, the condition we seek can be determined by evaluating Eq. (C5) in the Higgs basis.

With the help of *Mathematica*, we obtain the following results. In any basis,

$$[Z^{(1)}, Z^{(11)}]_{22} = -[Z^{(1)}, Z^{(11)}]_{11}, \quad \text{and} \quad [Z^{(1)}, Z^{(11)}]_{12} = -[Z^{(1)}, Z^{(11)}]_{21}^*. \quad (\text{C6})$$

In the Higgs basis,

$$[Z^{(1)}, Z^{(11)}]_{11} = 2i\{(Z_1 - Z_2)\text{Im}(Z_6^*Z_7) + \text{Im}(Z_5^*Z_6^2)\} = 0, \quad (\text{C7})$$

$$[Z^{(1)}, Z^{(11)}]_{12} = (Z_1 - Z_2)[Z_{34}Z_{67} - Z_2Z_6 - Z_1Z_7 + Z_5Z_6^*] - 2Z_{67}(|Z_6|^2 - |Z_7|^2), \quad (\text{C8})$$

where $Z_{34} \equiv Z_3 + Z_4$ and $Z_{67} \equiv Z_6 + Z_7$.

Thus, we arrive at two conditions for the Higgs basis scalar potential parameters that imply the existence of a softly broken Z_2 symmetry,

$$(Z_1 - Z_2)[Z_{34}Z_{67} - Z_2Z_6 - Z_1Z_7 + Z_5Z_{67}^*] - 2Z_{67}(|Z_6|^2 - |Z_7|^2) = 0, \quad (\text{C9})$$

$$(Z_1 - Z_2)\text{Im}(Z_6^*Z_7) + \text{Im}(Z_5^*Z_{67}^2) = 0, \quad (\text{C10})$$

which reproduce the results of Eqs. (89) and (88), respectively.

If the Z_2 symmetry is exact, then in addition to Eq. (C5), one must impose a second condition [33],

$$[Z^{(1)}, Y] = 0. \quad (\text{C11})$$

This result is established by evaluating the commutator in the Φ' basis where $\lambda'_7 = -\lambda'_6$. Noting that,

$$[Z^{(1)}, Y] = (\lambda'_2 - \lambda'_1) \begin{pmatrix} 0 & m_{12}^{\prime 2} \\ m_{12}^{\prime 2*} & 0 \end{pmatrix}, \quad (\text{C12})$$

it follows that if $\lambda'_1 \neq \lambda'_2$ and $m_{12}^{\prime 2} = 0$, then $[Z^{(1)}, Y] = 0$. That is, if Eqs. (C5) and (C11) are both satisfied and

$$Y^{(1)} = \begin{pmatrix} Y_1Z_1 + Y_3Z_6^* + Y_3^*Z_6 + Y_2Z_3 & Y_1Z_6 + Y_3Z_4 + Y_3^*Z_5 + Y_2Z_7 \\ Y_1Z_6^* + Y_3Z_5^* + Y_3^*Z_4 + Y_2Z_7^* & Y_1Z_3 + Y_3Z_7^* + Y_3^*Z_7 + Y_2Z_2 \end{pmatrix}. \quad (\text{C16})$$

If $Z_{67} = 0$ and $Z_1 = Z_2$, then we require that [33]

$$[Y^{(1)}, Y] = 0. \quad (\text{C17})$$

In the Higgs basis, Eq. (C17) yields

$$\begin{aligned} Y_3[Y_1(Z_3 - Z_1) + Y_3^*(Z_7 - Z_6) \\ + Y_3(Z_7^* - Z_6^*) + Y_2(Z_2 - Z_3)] \\ + (Y_1 - Y_2)(Y_1Z_6 + Y_3Z_4 + Y_3^*Z_5 + Y_2Z_7) = 0, \end{aligned} \quad (\text{C18})$$

$$Y_1\text{Im}(Y_3Z_6^*) + \text{Im}(Y_3^2Z_5^*) + Y_2\text{Im}(Y_3Z_7^*) = 0. \quad (\text{C19})$$

By assumption, $Z_{67} = 0$ and $Z_1 = Z_2$. The end result is

$$(Y_1 - Y_2) \left[Z_6^* \left(Y_2 + \frac{1}{2} Z_{34} v^2 \right) + \frac{1}{2} Z_6 Z_5^* v^2 \right] + Z_6^* |Z_6|^2 v^4 = 0, \quad (\text{C20})$$

$$\text{Im}(Z_5^* Z_6^2) = 0, \quad (\text{C21})$$

$\lambda'_1 \neq \lambda'_2$, then a basis exists where $m_{12}^{\prime 2} = \lambda'_6 = \lambda'_7 = 0$ and the Z_2 symmetry is manifest.

Evaluating Eq. (C11) in the Higgs basis,

$$\begin{pmatrix} Z_{14} & Z_{67} \\ Z_{67}^* & Z_{24} \end{pmatrix} \begin{pmatrix} Y_1 & Y_3 \\ Y_3^* & Y_2 \end{pmatrix} = \begin{pmatrix} Y_1 & Y_3 \\ Y_3^* & Y_2 \end{pmatrix} \begin{pmatrix} Z_{14} & Z_{67} \\ Z_{67}^* & Z_{24} \end{pmatrix}, \quad (\text{C13})$$

where we have again employed the notation, $Z_{ij} \equiv Z_i + Z_j$. This yields two conditions,

$$(Y_1 - Y_2)Z_{67}^* + Y_3^*(Z_2 - Z_1) = 0, \quad (\text{C14})$$

$$\text{Im}(Y_3^* Z_{67}) = 0, \quad (\text{C15})$$

which reproduces the results of Eqs. (125) and (124), respectively.

The exceptional region of parameter space (where $\lambda_7 = -\lambda_6$ and $\lambda_1 = \lambda_2$ in all scalar field bases) must be treated separately, Indeed Eqs. (C14) and (C15) are automatically satisfied, and additional considerations are warranted.

Following Ref. [33], we introduce $Y_{cd}^{(1)} \equiv Y_{b\bar{a}} Z_{a\bar{b}c\bar{d}}$, which is explicitly given in the Higgs basis by

after imposing the scalar potential minimum condition, $Y_3 = -\frac{1}{2}Z_6 v^2$ [cf. Eq. (24)].¹⁹ Multiplying Eq. (C20) by Z_6 yields

$$(Y_1 - Y_2) \left[|Z_6|^2 \left(Z_{34} + \frac{2Y_2}{v^2} \right) + Z_3^* Z_6^2 \right] + 2|Z_6|^4 v^2 = 0, \quad (\text{C22})$$

which reproduces Eq. (131). Indeed, the imaginary part of Eq. (C22) yields Eq. (C21), implying that the latter is not an independent condition.²⁰

APPENDIX D: PROOF OF THE EXISTENCE OF A SCALAR FIELD BASIS IN WHICH $\lambda'_7 = -\lambda'_6$

Starting from an arbitrary Φ basis of scalar fields, Eqs. (A2)–(A11) list the coefficients of the scalar potential

¹⁹In obtaining Eq. (C20), we made use of $Y_1Z_6 = Y_3Z_1$, which is a consequence of Eq. (24).

²⁰If $Y_1 = Y_2$, $Z_1 = Z_2$ and $Z_{67} = 0$, then Eq. (C20) implies that $Z_6 = 0$ and Eq. (C21) is trivially satisfied. Of course, in this case, the exact Z_2 symmetry is manifestly realized in the Higgs basis, and no further analysis is required.

in the Φ' basis that are related to the corresponding coefficients of the Φ basis by the $U(2)$ transformation given by Eq. (A1). It then follows that

$$(\lambda'_6 + \lambda'_7)e^{i\xi} = -\frac{1}{2}s_{2\beta}(\lambda_1 - \lambda_2) + c_{2\beta}\text{Re}[(\lambda_6 + \lambda_7)e^{i\xi}] + i\text{Im}[(\lambda_6 + \lambda_7)e^{i\xi}]. \quad (\text{D1})$$

We assume that $\lambda_7 \neq -\lambda_6$. The goal of this appendix is to show that there exists a choice of β and ξ such that $\lambda'_7 = -\lambda'_6$.

Consider the diagonalization of the matrix $Z_{ab}^{(1)} \equiv \delta_{c\bar{d}}Z_{a\bar{c}d\bar{b}}$, which is explicitly given by

$$Z^{(1)} \equiv \begin{pmatrix} \lambda_1 + \lambda_4 & \lambda_6 + \lambda_7 \\ \lambda_6^* + \lambda_7^* & \lambda_2 + \lambda_4 \end{pmatrix}. \quad (\text{D2})$$

Under a basis transformation, $\Phi_a \rightarrow \Phi'_a = U_{a\bar{b}}\Phi_b$, it follows that $Z_{ab}^{(1)} \rightarrow U_{a\bar{c}}Z_{c\bar{d}}^{(1)}U_{d\bar{b}}^\dagger$, where the unitary matrix U is given by Eq. (A1). It is possible to choose η , β , and ξ such that

$$UZ^{(1)}U^{-1} = \text{diag}(\lambda_+, \lambda_-), \quad (\text{D3})$$

where the λ_\pm are the eigenvalues of $Z^{(1)}$,

$$\lambda_\pm = \frac{1}{2} \left[\lambda_1 + \lambda_2 + 2\lambda_4 \pm \sqrt{(\lambda_1 - \lambda_2)^2 + 4|\lambda_6 + \lambda_7|^2} \right]. \quad (\text{D4})$$

In determining the diagonalization matrix U , one is free to take $\eta = 0$ without loss of generality.²¹ By convention, we shall also take $0 \leq \beta \leq \frac{1}{2}\pi$ and $0 \leq \xi < 2\pi$.

It is convenient to introduce the notation,

$$\lambda_{67} \equiv \lambda_6 + \lambda_7 \equiv |\lambda_{67}|e^{i\theta_{67}}. \quad (\text{D5})$$

It is then straightforward to check that the diagonalization of $Z^{(1)}$ is achieved if U is given by Eq. (A1) with $\eta = 0$, $\xi = -\theta_{67}$, and

$$s_{2\beta} = \frac{2|\lambda_{67}|}{\sqrt{(\lambda_1 - \lambda_2)^2 + 4|\lambda_{67}|^2}},$$

$$c_{2\beta} = \frac{\lambda_1 - \lambda_2}{\sqrt{(\lambda_1 - \lambda_2)^2 + 4|\lambda_{67}|^2}}, \quad (\text{D6})$$

Indeed, by inserting $\xi = -\theta_{67}$ into Eq. (D1) and using Eq. (D6), one readily verifies that

$$(\lambda'_6 + \lambda'_7)e^{i\xi} = -\frac{1}{2}s_{2\beta}(\lambda_1 - \lambda_2) + c_{2\beta}|\lambda_{67}| = 0, \quad (\text{D7})$$

after making use of Eq. (D6) in the final step. Hence, we conclude that $\lambda'_6 + \lambda'_7 = 0$. That is, it is always possible to find a basis change such that $\lambda'_6 = -\lambda'_7$.

For the record, we verify the diagonalization of $Z^{(1)}$ by computing

$$UZ^{(1)}U^{-1} = \begin{pmatrix} c_\beta & e^{i\theta_{67}}s_\beta \\ -e^{-i\theta_{67}}s_\beta & c_\beta \end{pmatrix} \begin{pmatrix} \lambda_1 + \lambda_4 & |\lambda_{67}|e^{i\theta_{67}} \\ |\lambda_{67}|e^{-i\theta_{67}} & \lambda_2 + \lambda_4 \end{pmatrix} \begin{pmatrix} c_\beta & -e^{-i\theta_{67}}s_\beta \\ e^{-i\theta_{67}}s_\beta & c_\beta \end{pmatrix}$$

$$= \begin{pmatrix} c_\beta & e^{i\theta_{67}}s_\beta \\ -e^{-i\theta_{67}}s_\beta & c_\beta \end{pmatrix} \begin{pmatrix} (\lambda_1 + \lambda_4)c_\beta + |\lambda_{67}|s_\beta & -e^{i\theta_{67}}[(\lambda_1 + \lambda_4)s_\beta - |\lambda_{67}|c_\beta] \\ e^{-i\theta_{67}}[|\lambda_{67}|c_\beta + (\lambda_2 + \lambda_4)s_\beta] & -|\lambda_{67}|s_\beta + (\lambda_2 + \lambda_4)c_\beta \end{pmatrix}. \quad (\text{D8})$$

In particular,

$$(UZ^{(1)}U^{-1})_{12} = (UZ^{(1)}U^{-1})_{21}^*$$

$$= e^{i\theta_{67}} \left[|\lambda_6 + \lambda_7|c_{2\beta} - \frac{1}{2}(\lambda_1 - \lambda_2)s_{2\beta} \right], \quad (\text{D9})$$

which vanishes if

$$\tan 2\beta = \frac{2|\lambda_{67}|}{\lambda_1 - \lambda_2}. \quad (\text{D10})$$

Note that this result is consistent with Eq. (D6).

²¹In light of Eq. (D3), it follows that the columns of $U^{-1} = U^\dagger$ are the normalized eigenvectors of $Z^{(1)}$, which are only defined up to an overall complex phase. Hence, one is free to rephase the second row of Eq. (A1) in order to set $\eta = 0$.

One can also check that $(UZ^{(1)}U^{-1})_{11} = \lambda_+$ and $(UZ^{(1)}U^{-1})_{22} = \lambda_-$, where

$$\lambda_\pm = \frac{1}{2}(\lambda_1 + \lambda_2 + 2\lambda_4) \pm \left[\frac{1}{2}(\lambda_1 - \lambda_2)c_{2\beta} + |\lambda_{67}|s_{2\beta} \right]. \quad (\text{D11})$$

Plugging in Eq. (D6) for $s_{2\beta}$ and $c_{2\beta}$ into Eq. (D11) then yields Eq. (D4), as expected.

APPENDIX E: MIXING OF THE NEUTRAL HIGGS SCALARS IN THE Φ BASIS

In Sec. III, the mixing of the neutral Higgs scalars was obtained in the Higgs basis. In this appendix, we examine the mixing in the Φ basis, where the scalar potential is given by Eq. (2). In the Φ basis, the two scalar doublet fields can be parametrized by

$$\Phi_1 = \begin{pmatrix} \varphi_1^+ \\ \frac{1}{\sqrt{2}}(v_1 + \eta_1 + i\chi_1) \end{pmatrix}, \quad \Phi_2 = e^{i\xi} \begin{pmatrix} \varphi_2^+ \\ \frac{1}{\sqrt{2}}(v_2 + \eta_2 + i\chi_2) \end{pmatrix}, \quad (\text{E1})$$

where

$$v_1 = v c_\beta, \quad v_2 = v s_\beta, \quad (\text{E2})$$

$c_\beta \equiv \cos \beta$, $s_\beta \equiv \sin \beta$, v is defined in Eq. (4), and the ranges of the parameters β and ξ are conventionally chosen to be $0 \leq \beta \leq \frac{1}{2}\pi$ and $0 \leq \xi < 2\pi$. The minimum conditions for the 2HDM scalar potential specified in Eq. (2) are

$$\begin{aligned} m_{11}^2 &= \text{Re}(m_{12}^2 e^{i\xi}) \tan \beta - \frac{1}{2} v^2 [\lambda_1 c_\beta^2 + \lambda_{345} s_\beta^2 + 3\text{Re}(\lambda_6 e^{i\xi}) s_\beta c_\beta + \text{Re}(\lambda_7 e^{i\xi}) s_\beta^2 \tan \beta], \\ m_{22}^2 &= \text{Re}(m_{12}^2 e^{i\xi}) \cot \beta - \frac{1}{2} v^2 [\lambda_2 s_\beta^2 + \lambda_{345} c_\beta^2 + \text{Re}(\lambda_6 e^{i\xi}) c_\beta^2 \cot \beta + 3\text{Re}(\lambda_7 e^{i\xi}) s_\beta c_\beta], \\ \text{Im}(m_{12}^2 e^{i\xi}) &= \frac{1}{2} v^2 [s_\beta c_\beta \text{Im}(\lambda_5 e^{2i\xi}) + \text{Im}(\lambda_6 e^{i\xi}) c_\beta^2 + \text{Im}(\lambda_7 e^{i\xi}) s_\beta^2], \end{aligned} \quad (\text{E3})$$

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

In light of Eqs. (21), (25), and (31), one can identify the neutral Goldstone boson with $G^0 = c_\beta \chi_1 + s_\beta \chi_2$ and the charged Goldstone boson with $G^\pm = c_\beta \varphi_1^\pm + s_\beta \varphi_2^\pm$. The neutral scalar state orthogonal to G^0 is denoted by η_3 and is given by

$$\eta_3 = c_\beta \chi_2 - s_\beta \chi_1. \quad (\text{E4})$$

An expression for the neutral Higgs mass-eigenstate fields was obtained in Eq. (37), which we repeat here for the convenience of the reader,

$$\begin{aligned} h_k &= \frac{1}{\sqrt{2}} [\bar{\Phi}_a^{0\dagger} (q_{k1} \hat{v}_a + q_{k2} \hat{w}_a e^{-i\theta_{23}}) \\ &\quad + (q_{k1}^* \hat{v}_a^* + q_{k2}^* \hat{w}_a^* e^{i\theta_{23}}) \bar{\Phi}_a^0], \end{aligned} \quad (\text{E5})$$

where the shifted neutral fields are defined by $\bar{\Phi}_a^0 \equiv \Phi_a^0 - v \hat{v}_a / \sqrt{2}$ and the $q_{k\ell}$ are exhibited in Table I. Plugging Eq. (E1) into Eq. (E5) yields

$$\begin{aligned} h_k &= (c_\beta \eta_1 + s_\beta \eta_2) \text{Re } q_{k1} + (c_\beta \chi_1 + s_\beta \chi_2) \text{Im } q_{k1} \\ &\quad + (c_\beta \eta_2 - s_\beta \eta_1) \text{Re}(q_{k2} e^{-i(\xi + \theta_{23})}) \\ &\quad + \eta_3 \text{Im}(q_{k2} e^{-i(\xi + \theta_{23})}), \end{aligned} \quad (\text{E6})$$

after employing Eq. (E4). Recall that for $k = 0$, we have $q_{01} = i$ and $q_{02} = 0$, in which case Eq. (E6) yields $h_0 = G^0$, as expected.

Making use of Eqs. (41) and (E5), the physical charged Higgs field is given by

$$H^\pm = e^{i(\xi + \theta_{23})} (c_\beta \varphi_2^\pm - s_\beta \varphi_1^\pm). \quad (\text{E7})$$

Focusing next on the three physical neutral Higgs bosons, h_k (for $k = 1, 2, 3$), we introduce the neutral Higgs mixing matrix, \mathcal{R} [cf. Eqs. (140) and (141)],

$$h_k = \mathcal{R}_{k\ell} \eta_\ell, \quad \text{for } k = 1, 2, 3. \quad (\text{E8})$$

where there is an implicit sum over the repeated index ℓ . Comparing Eqs. (E6) and (E8) and recalling that the q_{k1} are real for $k = 1, 2, 3$, it immediately follows that

$$\mathcal{R}_{k1} = q_{k1} c_\beta - \text{Re}(q_{k2} e^{-i(\xi + \theta_{23})}) s_\beta, \quad (\text{E9})$$

$$\mathcal{R}_{k2} = q_{k1} s_\beta + \text{Re}(q_{k2} e^{-i(\xi + \theta_{23})}) c_\beta, \quad (\text{E10})$$

$$\mathcal{R}_{k3} = \text{Im}(q_{k2} e^{-i(\xi + \theta_{23})}). \quad (\text{E11})$$

Not surprisingly, the individual elements of the matrix \mathcal{R} are basis dependent, since there is no physical meaning to the parameters β and ξ if the 2HDM Lagrangian possesses no Higgs family symmetry (beyond a global U(1) hypercharge). Nevertheless, one can construct combinations of the matrix elements of \mathcal{R} that are invariant or pseudoinvariant with respect to U(2)-basis transformations. For example,

$$q_{k1} = \mathcal{R}_{k1} c_\beta + \mathcal{R}_{k2} s_\beta, \quad (\text{E12})$$

$$q_{k2} e^{-i(\xi + \theta_{23})} = -\mathcal{R}_{k1} s_\beta + \mathcal{R}_{k2} c_\beta + i \mathcal{R}_{k3}. \quad (\text{E13})$$

Indeed, the above combinations appear in the gauge boson–Higgs boson couplings [32].²²

²²The combination of matrix elements on the right-hand side of Eq. (E13) appears in the couplings of the charged Higgs boson. The factor of $e^{-i(\xi + \theta_{23})}$ that multiplies the invariant quantity q_{k2} in Eq. (E13) cancels against the phase factor appearing in Eq. (E7), resulting in charged Higgs couplings that are invariant with respect to U(2)-basis transformations, as expected for the physical couplings of invariant fields.

All the results above also apply in the 2HDM with a softly broken \mathbb{Z}_2 symmetry, where $\lambda_6 = \lambda_7 = 0$ in the Φ basis. In this case, we may use the results of Sec. V B. In particular, both $c_{2\beta}$ and $e^{-i(\xi+\theta_{23})}$ are now determined up to a twofold ambiguity by Eqs. (82) and (84), respectively, in terms of basis-invariant quantities. This twofold ambiguity corresponds to a residual basis dependence associated with the interchange of the two scalar fields. Under the interchange of $\Phi_1 \leftrightarrow \Phi_2$, it follows from Eqs. (72) to (75) that $e^{i(\xi+\theta_{23})} \rightarrow -e^{i(\xi+\theta_{23})}$ and $s_\beta \leftrightarrow c_\beta$, in which case Eqs. (E9)–(E11) imply that $\mathcal{R}_{k1} \leftrightarrow \mathcal{R}_{k2}$ and $\mathcal{R}_{k3} \rightarrow -\mathcal{R}_{k3}$.

However, θ_{23} and ξ are not separately determined. This is not surprising since θ_{23} and ξ are each additively shifted by a rephasing of the second Higgs doublet of the \mathbb{Z}_2 basis and the Φ basis, respectively. Nevertheless, the presence of the softly broken \mathbb{Z}_2 symmetry ties these two parameter shifts together such that their sum $\xi + \theta_{23}$ is invariant under a rephasing of the corresponding scalar doublets. Indeed, the fact that only the sum $\xi + \theta_{23}$ appears in Eq. (E7) and in Eqs. (E9)–(E11) could have been anticipated on these grounds.

Using Eqs. (E9)–(E11), one can now derive a useful sum rule,

$$\begin{aligned} \frac{1}{v^2} \sum_{k=1}^3 m_k^2 \mathcal{R}_{k3} (\mathcal{R}_{k1} c_\beta - \mathcal{R}_{k2} s_\beta) &= \frac{1}{v^2} c_{2\beta} \sum_{k=1}^3 m_k^2 q_{k1} \text{Im}(q_{k2} e^{-i(\xi+\theta_{23})}) - \frac{1}{2v^2} s_\beta \sum_{k=1}^3 m_k^2 \text{Im}(q_{k2}^2 e^{-2i(\xi+\theta_{23})}) \\ &= -c_{2\beta} \text{Im}(Z_6 e^{i\xi}) + \frac{1}{2} s_{2\beta} \text{Im}(Z_5 e^{2i\xi}), \end{aligned} \quad (\text{E14})$$

after making use of Eqs. (49) and (50). Since $\lambda_6 = \lambda_7 = 0$ in the \mathbb{Z}_2 basis, one can employ Eqs. (A9) and (A10) to obtain²³

$$\text{Im}(Z_5 e^{2i\xi}) = c_{2\beta} \text{Im}(\lambda_5 e^{2i\xi}), \quad \text{Im}(Z_6 e^{i\xi}) = \frac{1}{2} s_{2\beta} \text{Im}(\lambda_5 e^{2i\xi}). \quad (\text{E15})$$

Inserting these results into Eq. (E14) yields²⁴

$$\sum_{k=1}^3 m_k^2 \mathcal{R}_{k3} (\mathcal{R}_{k1} c_\beta - \mathcal{R}_{k2} s_\beta) = 0. \quad (\text{E16})$$

Note that this sum rule is independent of the parameter ξ .

After setting $\lambda_6 = \lambda_7 = 0$ in Eq. (E3), m_{11}^2 , m_{22}^2 , and $\text{Im}(m_{12}^2 e^{i\xi})$ are then fixed by the scalar potential minimum conditions. Hence, it follows that the most general 2HDM subject to a softly broken \mathbb{Z}_2 symmetry is governed by nine independent parameters that can be identified by using Eq. (E16) to impose one relation among the ten real quantities: v , $\tan\beta$, $\text{Re}(m_{12}^2 e^{i\xi})$, three mixing angles, three neutral Higgs masses, and one charged Higgs mass.

²³When using Eqs. (A10) and (A11), we identify the coefficients of the Higgs basis scalar potential given by Eq. (28); e.g., $\lambda'_5 = Z_5 e^{-2i\eta}$ and $\lambda'_6 = Z_6 e^{-i\eta}$. Thus, the factors of η cancel out in obtaining Eq. (E15).

²⁴Equation (E16) first appears explicitly in Ref. [60].

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- [1] T. D. Lee, *Phys. Rev. D* **8**, 1226 (1973); *Phys. Rep.* **9**, 143 (1974).
 - [2] R. D. Peccei and H. R. Quinn, *Phys. Rev. Lett.* **38**, 1440 (1977).
 - [3] P. Fayet, *Nucl. Phys.* **B78**, 14 (1974).
 - [4] K. Inoue, A. Kakuto, H. Komatsu, and S. Takeshita, *Prog. Theor. Phys.* **67**, 1889 (1982).
 - [5] R. A. Flores and M. Sher, *Ann. Phys. (N.Y.)* **148**, 95 (1983).
 - [6] J. F. Gunion and H. E. Haber, *Nucl. Phys.* **B272**, 1 (1986); **278**, 449 (1986); **402**, 567(E) (1993).
 - [7] J. F. Gunion, H. E. Haber, G. Kane, and S. Dawson, *The Higgs Hunter's Guide* (Westview Press, Boulder, CO, 2000).
 - [8] F. J. Botella and J. P. Silva, *Phys. Rev. D* **51**, 3870 (1995).
 - [9] G. C. Branco, L. Lavoura, and J. P. Silva, *CP Violation* (Oxford University Press, Oxford, United Kingdom, 1999), Chaps. 22 and 23.
 - [10] M. Carena and H. E. Haber, *Prog. Part. Nucl. Phys.* **50**, 63 (2003).
 - [11] A. Djouadi, *Phys. Rep.* **457**, 1 (2008); **459**, 1 (2008).
 - [12] G. C. Branco, P. M. Ferreira, L. Lavoura, M. N. Rebelo, M. Sher, and J. P. Silva, *Phys. Rep.* **516**, 1 (2012).
 - [13] S. L. Glashow and S. Weinberg, *Phys. Rev. D* **15**, 1958 (1977).
 - [14] E. A. Paschos, *Phys. Rev. D* **15**, 1966 (1977).
 - [15] H. Georgi and D. V. Nanopoulos, *Phys. Lett.* **82B**, 95 (1979).
 - [16] J. F. Gunion and H. E. Haber, *Phys. Rev. D* **67**, 075019 (2003).

- [17] N. Craig, J. Galloway, and S. Thomas, [arXiv:1305.2424](#).
- [18] H. E. Haber, in *Proceedings of the of the Toyama International Workshop on Higgs as a Probe of New Physics 2013 (HPNP2013)*, [arXiv:1401.0152](#).
- [19] D. M. Asner *et al.*, [arXiv:1310.0763](#).
- [20] M. Carena, I. Low, N. R. Shah, and C. E. M. Wagner, *J. High Energy Phys.* **04** (2014) 015.
- [21] P. S. Bhupal Dev and A. Pilaftsis, *J. High Energy Phys.* **12** (2014) 024; **11** (2015) 147(E).
- [22] D. Das and I. Saha, *Phys. Rev. D* **91**, 095024 (2015).
- [23] B. Grzadkowski, H. E. Haber, O. M. Ogreid, and P. Osland, *J. High Energy Phys.* **12** (2018) 056.
- [24] I. F. Ginzburg, M. Krawczyk, and P. Osland, in *Proceedings of the International Workshop on Physics and Experiments with Future Electron-Positron Linear Colliders, LCWS 2002, Seogwipo, Jeju Island, Korea, 2002*, edited by J. S. Kang and S. K. Oh (Sorim Press, 2003), pp. 703–706, [arXiv:hep-ph/0211371](#).
- [25] I. F. Ginzburg and M. Krawczyk, *Phys. Rev. D* **72**, 115013 (2005).
- [26] A. W. El Kaffas, W. Khater, O. M. Ogreid, and P. Osland, *Nucl. Phys.* **B775**, 45 (2007).
- [27] A. Arhrib, E. Christova, H. Eberl, and E. Ginina, *J. High Energy Phys.* **04** (2011) 089.
- [28] A. Barroso, P. M. Ferreira, R. Santos, and J. P. Silva, *Phys. Rev. D* **86**, 015022 (2012).
- [29] S. Inoue, M. J. Ramsey-Musolf, and Y. Zhang, *Phys. Rev. D* **89**, 115023 (2014).
- [30] D. Fontes, J. C. Romão, and J. P. Silva, *J. High Energy Phys.* **12** (2014) 043.
- [31] B. Grzadkowski, O. M. Ogreid, and P. Osland, *J. High Energy Phys.* **11** (2014) 084.
- [32] D. Fontes, M. Mühlleitner, J. C. Romão, R. Santos, J. P. Silva, and J. Wittbrodt, *J. High Energy Phys.* **02** (2018) 073.
- [33] S. Davidson and H. E. Haber, *Phys. Rev. D* **72**, 035004 (2005); **72**, 099902(E) (2005).
- [34] H. E. Haber and D. O’Neil, *Phys. Rev. D* **74**, 015018 (2006); **74**, 059905(E) (2006).
- [35] B. Grzadkowski, O. M. Ogreid, and P. Osland, *Phys. Rev. D* **94**, 115002 (2016).
- [36] I. P. Ivanov, *Phys. Lett. B* **632**, 360 (2006).
- [37] C. C. Nishi, *Phys. Rev. D* **74**, 036003 (2006); **76**, 119901(E) (2007).
- [38] M. Maniatis, A. von Manteuffel, and O. Nachtmann, *Eur. Phys. J. C* **57**, 719 (2008).
- [39] P. M. Ferreira, M. Maniatis, O. Nachtmann, and J. P. Silva, *J. High Energy Phys.* **08** (2010) 125.
- [40] P. M. Ferreira, H. E. Haber, M. Maniatis, O. Nachtmann, and J. P. Silva, *Int. J. Mod. Phys. A* **26**, 769 (2011).
- [41] I. P. Ivanov, C. C. Nishi, and A. Trautner, *Eur. Phys. J. C* **79**, 315 (2019).
- [42] H. E. Haber, G. L. Kane, and T. Sterling, *Nucl. Phys.* **B161**, 493 (1979).
- [43] J. F. Donoghue and L. F. Li, *Phys. Rev. D* **19**, 945 (1979).
- [44] L. J. Hall and M. B. Wise, *Nucl. Phys.* **B187**, 397 (1981).
- [45] H. E. Haber and O. Stål, *Eur. Phys. J. C* **75**, 491 (2015); **76**, 312(E) (2016).
- [46] L. Lavoura, *Phys. Rev. D* **50**, 7089 (1994).
- [47] P. M. Ferreira, H. E. Haber, and J. P. Silva, *Phys. Rev. D* **79**, 116004 (2009).
- [48] L. Lavoura and J. P. Silva, *Phys. Rev. D* **50**, 4619 (1994).
- [49] H. E. Haber and D. O’Neil, *Phys. Rev. D* **83**, 055017 (2011).
- [50] H. Huffel and G. Pocsik, *Z. Phys. C* **8**, 13 (1981).
- [51] H. A. Weldon, *Phys. Rev. D* **30**, 1547 (1984).
- [52] A. G. Akeroyd, A. Arhrib, and E. M. Naimi, *Phys. Lett. B* **490**, 119 (2000).
- [53] I. F. Ginzburg and I. P. Ivanov, *Phys. Rev. D* **72**, 115010 (2005).
- [54] J. Horejsi and M. Kladiva, *Eur. Phys. J. C* **46**, 81 (2006).
- [55] S. Kanemura and K. Yagyu, *Phys. Lett. B* **751**, 289 (2015).
- [56] M. Nebot, [arXiv:1911.02266](#).
- [57] H. E. Haber and J. P. Silva (to be published).
- [58] H. Bélusca-Maïto, A. Falkowski, D. Fontes, J. C. Romão, and J. P. Silva, *J. High Energy Phys.* **04** (2018) 002.
- [59] J. F. Guinon and H. E. Haber, *Phys. Rev. D* **72**, 095002 (2005).
- [60] A. W. El Kaffas, P. Osland, and O. M. Ogreid, *Nonlin. Phenom. Complex Syst.* **10**, 347 (2007), <https://arxiv.org/abs/hep-ph/0702097>.
- [61] D. Fontes, M. Mühlleitner, J. C. Romão, R. Santos, J. P. Silva, and J. Wittbrodt, *Couplings of the C2HDM*, <http://porthos.tecnico.ulisboa.pt/arXiv/C2HDM/> (2017).
- [62] G. C. Branco and M. N. Rebelo, *Phys. Lett.* **160B**, 117 (1985).
- [63] G. C. Branco, M. N. Rebelo, and J. I. Silva-Marcos, *Phys. Lett. B* **614**, 187 (2005).
- [64] P. M. Ferreira and J. P. Silva, *Eur. Phys. J. C* **69**, 45 (2010).