Basis-independent methods for the two-Higgs-doublet model. II. The significance of $\tan\beta$

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In the most general two-Higgs-doublet model (2HDM), there is no distinction between the two complex hypercharge-one $SU(2)_L$ doublet scalar fields, Φ_a ($a = 1, 2$). Thus, any two orthonormal linear combinations of these two fields can serve as a basis for the Lagrangian. All physical observables of the model must be basis-independent. For example, $\tan\beta \equiv \langle\Phi_2^0\rangle/\langle\Phi_1^0\rangle$ is basis-dependent and thus cannot be a physical parameter of the model. In this paper, we provide a basis-independent treatment of the Higgs sector with particular attention to the neutral Higgs boson mass-eigenstates, which generically are *not* eigenstates of CP. We then demonstrate that all physical Higgs couplings are indeed independent of $\tan\beta$. In specialized versions of the 2HDM, $\tan\beta$ can be promoted to a physical parameter of the Higgs-fermion interactions. In the most general 2HDM, the Higgs-fermion couplings can be expressed in terms of a number of physical "$\tan\beta$-like" parameters that are manifestly basis-independent. The minimal supersymmetric extension of the standard model provides a simple framework for exhibiting such effects.

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I. INTRODUCTION

The two-Higgs-doublet model (2HDM) is one of the most well studied extensions of the standard model. Various motivations for adding a second hypercharge-one complex Higgs doublet to the standard model have been advocated in the literature [1–7]. Perhaps the best motivated of these two-Higgs-doublet models is the minimal supersymmetric extension of the standard model (MSSM) [8], which requires a second Higgs doublet (and its supersymmetric fermionic partners) in order to preserve the cancellation of gauge anomalies.

In most cases, the structure of the 2HDM is constrained in some way. For example, in many of the early two-Higgs-doublet models proposed in the literature, a discrete symmetry was introduced that restricted the most general form of the Higgs scalar potential and the Higgs-fermion interactions [9–13]. In the MSSM, this discrete symmetry is not present, but the imposition of supersymmetry on the dimension-four terms of the Lagrangian yields similar restrictions on the Higgs-fermion interactions and even more stringent restrictions on the scalar potential.

It is tempting to relax these constraints and study the most general 2HDM consistent with the electroweak $SU(2)_L \times U(1)_Y$ gauge symmetry. However, phenomenology dictates that we choose the Higgs-fermion interactions with some care [14,15] to avoid neutral Higgs-mediated flavor-changing neutral currents (FCNCs) at tree level. In the most general 2HDM, these effects are present, and can only be suppressed (to avoid conflict with observed data) by a significant fine-tuning of the Higgs-fermion interactions (to ensure that certain couplings are small enough in magnitude). Theoretically, it is more natural to introduce a symmetry to completely remove the tree-level FCNC effects. Both the discrete symmetries alluded to above and supersymmetry provide just such a natural mechanism.

Nevertheless, symmetries are often broken. Supersymmetry is not an exact symmetry, and it is possible to imagine small violations of the discrete symmetries generated from new physics at the TeV-scale. In both cases, when the TeV-scale physics is integrated out, the effective low-energy theory can resemble the most general 2HDM, albeit with small couplings of the dangerous interactions that can potentially yield tree-level FCNC effects.

The LHC will soon provide the first comprehensive look at the TeV-scale. Experiments from this collider may yield the first hints of the existence of a nonminimal Higgs sector. Precision Higgs studies are one of the primary motivations for the development of the International Linear Collider (ILC) [16]. Data from the ILC could provide detailed evidence of a 2HDM structure responsible for electroweak symmetry breaking. To make further progress, one must measure the Higgs sector observables with some precision in order to reconstruct (as best as one can) the Higgs Lagrangian. Given that we will not know *a priori* the theoretical principles that constrain the Higgs sector, it is critical to develop techniques for identifying experimental observables with the physical parameter of the model. In this context, a *physical* parameter is one that is measurable (in principle) without imposing any simplifying theoretical assumptions.

Perhaps the simplest example of an unphysical parameter of the 2HDM is the well-known quantity

$$\tan\beta \equiv \frac{\langle\Phi_2^0\rangle}{\langle\Phi_1^0\rangle}, \tag{1}$$

given by the ratio of the two neutral Higgs field vacuum expectation values. The problem with this quantity is that its definition assumes that one can distinguish between the two *identical* hypercharge-one-Higgs-doublet fields. In the most general 2HDM, there is no preferred choice of *basis* of scalar fields $\Phi_1 - \Phi_2$. Any two sets of scalar doublets related by a global 2×2 unitary transformation are equally valid choices. Clearly, $\tan\beta$ is a basis-dependent quantity, and hence is not a physical parameter. Only basis-independent quantities can be physical.

In the more specialized 2HDMs, a preferred basis is singled out. For example, in the models with discrete symmetries and in the MSSM, the Higgs potential exhibits a special form in the preferred basis. Then $\tan\beta$ can be defined with respect to this basis and thereby is promoted to a physical parameter. However, if we allow for symmetry-breaking effects, the effective low-energy theory is a completely general 2HDM (albeit with certain relations inherited from the more fundamental theory). In this case, the identification of $\tan\beta$ as a physical parameter is more subtle. Moreover, in order to perform truly model-independent analyses of the Higgs precision data, one should refrain from any additional theoretical assumptions, in which case $\tan\beta$ once again is relegated to the class of basis-dependent (and hence unphysical) parameters.

In Ref. [17], a basis-independent formalism was advocated in order to avoid the potential problems associated with unphysical parameters. In particular, the importance of a basis-independent form for all Higgs couplings was stressed. These are the quantities that one wishes to extract from precision Higgs experiments. For example, in the case of the Higgs-fermion interactions, the parameter $\tan\beta$ never appears. Instead, one can identify various basis-independent $\tan\beta$-like parameters that can be identified with ratios of physical couplings. One of the main shortcomings of Ref. [17] is that this program was only carried out in the approximation of a CP-conserving scalar potential. However, in the most general 2HDM, the scalar potential possesses complex couplings that can generate CP-violating effects. Among the most important of these effects is the mixing of CP-even and CP-odd scalar eigenstates to produce neutral Higgs mass-eigenstates of indefinite CP quantum numbers. In this paper, we complete the analysis of Ref. [17] by identifying the basis-independent form for the Higgs couplings, allowing for the most general CP-violating effects.

In Sec. II, we review the basis-independent formalism of Ref. [17]. This formalism was inspired by an elegant presentation of the 2HDM in Ref. [7]. Although any basis choice is as good as any other basis choice, the Higgs basis (defined to be a basis in which one of the two neutral scalar fields has zero vacuum expectation value) possesses some invariant features. In Sec. III, we review the construction of the Higgs basis and use the basis-independent formalism to highlight the invariant qualities of this basis choice. Ultimately, we are interested in the Higgs mass-eigenstates. In the most general CP-violating 2HDM, three neutral Higgs states mix to form mass-eigenstates that are not eigenstates of CP. In Sec. IV, we demonstrate how to define basis-independent Higgs mixing parameters that are crucial for deriving an invariant form for the Higgs couplings.

In Sec. V and VI we provide the explicit basis-independent forms for the Higgs couplings to bosons (gauge bosons and Higgs boson self-couplings) and fermions (quarks and leptons), respectively. Finally, in Sec. VII we return to the question of the significance of $\tan\beta$. We demonstrate in a one-generation model how to define three basis-independent $\tan\beta$-like parameters in terms of physical Higgs-fermion couplings. In special cases, these three parameters all reduce to the usual $\tan\beta$. However, in the most general case, these three parameters can differ. The detection of such differences would yield important clues to the fundamental nature of the 2HDM theoretical structure. Conclusions and an outlook to future work are addressed in section VIII. Some additional details are relegated to a set of four appendices. In particular, Appendix D provides the link between the most general 2HDM considered in this paper and the more common CP-conserving 2HDM that is often treated in the literature.

The basis-independent formalism has attracted some attention during the past year. In Refs. [17–20], these techniques have been exploited to great advantage in the study of the CP-violating structure of the 2HDM (and extend the results originally obtained in Refs. [21,22]). In addition, the importance of the global U(2) transformation of the two-Higgs-doublet fields (and the subgroup of $U(1) \times U(1)$ rephasing transformations) has been emphasized, and some of their implications for 2HDM phenomenology have been explored recently in Ref. [23].

II. THE BASIS-INDEPENDENT FORMALISM

The fields of the two-Higgs-doublet model (2HDM) consist of two identical complex hypercharge-one, $SU(2)_L$ doublet scalar fields $\Phi_a(x) \equiv (\Phi_a^+(x), \Phi_a^0(x))$, where $a = 1, 2$ labels the two-Higgs-doublet fields, and will be referred to as the Higgs "flavor" index. The Higgs-doublet fields can always be redefined by an arbitrary nonsingular complex transformation $\Phi_a \to B_{ab}\Phi_b$, where the matrix B depends on eight real parameters. However, four of these parameters can be used to transform the scalar field kinetic energy terms into canonical form.[1] The most general redefinition of the scalar fields [which leaves invariant the form of the canonical kinetic energy terms $\mathcal{L}_{\rm KE} = (D_\mu\Phi)^\dagger_{\bar{a}}(D^\mu\Phi)_a$] corresponds to a global $U(2)$ transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$ [and $\Phi^\dagger_{\bar{a}} \to \Phi^\dagger_{\bar{b}} U^\dagger_{b\bar{a}}$], where the 2×2 unitary matrix U satisfies $U^\dagger_{b\bar{a}} U_{a\bar{c}} = \delta_{b\bar{c}}$. In our index conventions, replacing an unbarred index with a barred index is equivalent to complex conjugation. We

[1]That is, starting from $\mathcal{L}_{\rm KE} = a(D_\mu\Phi_1)^\dagger(D_\mu\Phi_1) + b(D_\mu\Phi_2)^\dagger(D_\mu\Phi_2) + [c(D_\mu\Phi_1)^\dagger(D_\mu\Phi_2) + \text{H.c.}]$, where a and b are real and c is complex, one can always find a (nonunitary) transformation B that removes the four real degrees of freedom corresponding to a, b, and c and sets $a = b = 1$ and $c = 0$. Mathematically, such a transformation is an element of the coset space $GL(2, \mathbb{C})/U(2)$.

only allow sums over barred-unbarred index pairs, which are performed by employing the U(2)-invariant tensor $\delta_{a\bar{b}}$. The basis-independent formalism consists of writing all equations involving the Higgs sector fields in a U(2)-covariant form. Basis-independent quantities can then be identified as U(2)-invariant scalars, which are easily identified as products of tensor quantities with all barred-unbarred index pairs summed with no Higgs flavor indices left over.

We begin with the most general 2HDM scalar potential. An explicit form for the scalar potential in a generic basis is given in Appendix A. Following Refs. [7,17], the scalar potential can be written in U(2)-covariant form:

$$\mathcal{V} = Y_{a\bar{b}}\Phi_{\bar{a}}^{\dagger}\Phi_b + \tfrac{1}{2}Z_{a\bar{b}c\bar{d}}(\Phi_{\bar{a}}^{\dagger}\Phi_b)(\Phi_{\bar{c}}^{\dagger}\Phi_d), \tag{2}$$

where the indices a, $\bar{b}$, c, and $\bar{d}$ are labels with respect to the two-dimensional Higgs flavor space and $Z_{a\bar{b}c\bar{d}} = Z_{c\bar{d}a\bar{b}}$. The hermiticity of $\mathcal{V}$ yields $Y_{a\bar{b}} = (Y_{b\bar{a}})^*$ and $Z_{a\bar{b}c\bar{d}} = (Z_{b\bar{a}d\bar{c}})^*$. Under a U(2) transformation, the tensors $Y_{a\bar{b}}$ and $Z_{a\bar{b}c\bar{d}}$ transform covariantly: $Y_{a\bar{b}} \to U_{a\bar{c}}Y_{c\bar{d}}U_{d\bar{b}}^{\dagger}$ and $Z_{a\bar{b}c\bar{d}} \to U_{a\bar{e}}U_{f\bar{b}}^{\dagger}U_{c\bar{g}}U_{h\bar{d}}^{\dagger}Z_{e\bar{f}g\bar{h}}$. Thus, the scalar potential $\mathcal{V}$ is a U(2)-scalar. The interpretation of these results is simple. Global U(2)-flavor transformations of the two Higgs doublet fields do not change the functional form of the scalar potential. However, the coefficients of each term of the potential depends on the choice of basis. The transformation of these coefficients under a U(2) basis change are precisely the transformation laws of Y and Z given above.

We shall assume that the vacuum of the theory respects the electromagnetic $\mathrm{U}(1)_{\mathrm{EM}}$ gauge symmetry. In this case, the nonzero vacuum expectation values of Φ_a must be aligned. The standard convention is to make a gauge-$\mathrm{SU}(2)_{\mathrm{L}}$ transformation (if necessary) such that the lower (or second) component of the doublet fields correspond to electric charge $Q = 0$. In this case, the most general $\mathrm{U}(1)_{\mathrm{EM}}$-conserving vacuum expectation values are

$$\langle\Phi_a\rangle = \frac{v}{\sqrt{2}}\begin{pmatrix} 0 \\ \hat{v}_a \end{pmatrix} \quad \text{with} \quad \hat{v}_a \equiv e^{i\eta}\begin{pmatrix} c_\beta \\ s_\beta e^{i\xi} \end{pmatrix}, \tag{3}$$

where $v \equiv 2m_W/g = 246$ GeV and $\hat{v}_a$ is a vector of unit norm. The overall phase η is arbitrary. By convention, we take $0 \leq \beta \leq \pi/2$ and $0 \leq \xi < 2\pi$. Taking the derivative of Eq. (2) with respect to Φ_b, and setting $\langle\Phi_a^0\rangle = v_a/\sqrt{2}$, we find the covariant form for the scalar potential minimum conditions:

$$v\hat{v}_{\bar{a}}^*[Y_{a\bar{b}} + \tfrac{1}{2}v^2 Z_{a\bar{b}c\bar{d}}\hat{v}_{\bar{c}}^*\hat{v}_d] = 0. \tag{4}$$

Before proceeding, let us consider the most general global-U(2) transformation (see p. 5 of Ref. [24]):

$$U = e^{i\psi}\begin{pmatrix} e^{i\gamma}\cos\theta & e^{-i\zeta}\sin\theta \\ -e^{i\zeta}\sin\theta & e^{-i\gamma}\cos\theta \end{pmatrix}, \tag{5}$$

where $-\pi \leq \theta, \psi < \pi$, and $-\pi/2 \leq \zeta, \gamma \leq \pi/2$ defines the closed and bounded U(2) parameter space. If we fix $\psi = 0$, then the U span an SU(2) matrix subgroup of U(2), and $\{e^{i\psi}\}$ constitutes a U(1) subgroup of U(2). More precisely, $\mathrm{U}(2) \cong \mathrm{SU}(2) \times \mathrm{U}(1)/\mathbb{Z}_2$. In the scalar sector, this U(1) coincides with global hypercharge $\mathrm{U}(1)_{\mathrm{Y}}$. However, the former U(1) is distinguished from hypercharge by the fact that it has no effect on the other fields of the standard model.

Because the scalar potential is *invariant* under $\mathrm{U}(1)_{\mathrm{Y}}$ hypercharge transformations,[2] it follows that Y and Z are invariant under U(1)-flavor transformations. Thus, from the standpoint of the Lagrangian, only SU(2)-flavor transformations correspond to a change of basis. Nevertheless, the vacuum expectation value $\hat{v}$ does change by an overall phase under flavor-U(1) transformations. Thus, it is convenient to expand our definition of the basis to include the phase of $\hat{v}$. In this convention, all U(2)-flavor transformations correspond to a change of basis. The reason for this choice is that it permits us to expand our potential list of basis-independent quantities to include quantities that depend on $\hat{v}$. Since $\Phi_a \to U_{a\bar{b}}\Phi_b$ it follows that $\hat{v}_a \to U_{a\bar{b}}\hat{v}_b$, and the covariance properties of quantities that depend on $\hat{v}$ are easily discerned.

The unit vector $\hat{v}_a$ can also be regarded as an eigenvector of unit norm of the Hermitian matrix $V_{a\bar{b}} \equiv \hat{v}_a\hat{v}_{\bar{b}}^*$. The overall phase of $\hat{v}_a$ is not determined in this definition, but as noted above different phase choices are related by U(1)-flavor transformations. Since $V_{a\bar{b}}$ is Hermitian, it possesses a second eigenvector of unit norm that is orthogonal to $\hat{v}_a$. We denote this eigenvector by $\hat{w}_a$, which satisfies:

$$\hat{v}_{\bar{b}}^*\hat{w}_b = 0. \tag{6}$$

The most general solution to Eq. (6), up to an overall multiplicative phase factor, is

$$\hat{w}_b \equiv \hat{v}_{\bar{a}}^*\epsilon_{ab} = e^{-i\eta}\begin{pmatrix} -s_\beta e^{-i\xi} \\ c_\beta \end{pmatrix}. \tag{7}$$

That is, we have chosen a convention in which $\hat{w}_b \equiv e^{i\chi}\hat{v}_{\bar{a}}^*\epsilon_{ab}$, where $\chi = 0$. Of course, χ is not fixed by Eq. (6); the existence of this phase choice is reflected in the nonuniqueness of the Higgs basis, as discussed in Sec. III.

The inverse relation to Eq. (7) is easily obtained: $\hat{v}_{\bar{a}}^* = \epsilon_{\bar{a}\bar{b}}\hat{w}_b$. Above, we have introduced two Levi-Civita tensors with $\epsilon_{12} = -\epsilon_{21} = 1$ and $\epsilon_{11} = \epsilon_{22} = 0$. However, ϵ_{ab} and $\epsilon_{\bar{a}\bar{b}}$ are not proper tensors with respect to the flavor-U(2) group [although these are invariant SU(2)-tensors]. Consequently, $\hat{w}_a$ does not transform covariantly with respect to the full flavor-U(2) group. If we write $U = e^{i\psi}\hat{U}$, with $\det\hat{U} = 1$ (and $\det U = e^{2i\psi}$), it is simple to check that under a U(2) transformation

[2] The $\mathrm{SU}(2)_{\mathrm{L}} \times \mathrm{U}(1)_{\mathrm{Y}}$ gauge transformations act on the fields of the standard model, but do *not* transform the coefficients of the terms appearing in the Lagrangian.

$$\hat{v}_a \longrightarrow U_{a\bar{b}}\hat{v}_b \text{ implies that } \hat{w}_a \longrightarrow (\det U)^{-1}U_{a\bar{b}}\hat{w}_b. \quad (8)$$

Henceforth, we shall define a pseudotensor[3] as a tensor that transform covariantly with respect to the flavor-SU(2) subgroup but whose transformation law with respect to the full flavor-U(2) group is only covariant modulo an overall nontrivial phase equal to some integer power of $\det U$. Thus, $\hat{w}_a$ is a pseudovector. However, we can use $\hat{w}_a$ to construct proper tensors. For example, the Hermitian matrix $W_{a\bar{b}} \equiv \hat{w}_a\hat{w}^*_{\bar{b}} = \delta_{a\bar{b}} - V_{a\bar{b}}$ is a proper second-ranked tensor.

Likewise, a pseudoscalar (henceforth referred to as a pseudoinvariant) is defined as a quantity that transforms under U(2) by multiplication by some integer power of $\det U$. We reiterate that pseudoinvariants *cannot* be physical observables as the latter must be true U(2)-invariants.

III. THE HIGGS BASES

Once the scalar potential minimum is determined, which defines $\hat{v}_a$, one class of basis choices is uniquely selected. Suppose we begin in a generic $\Phi_1 - \Phi_2$ basis. We define new Higgs-doublet fields:

$$\begin{aligned} H_1 &= (H_1^+, H_1^0) \equiv \hat{v}^*_{\bar{a}}\Phi_a, \\ H_2 &= (H_2^+, H_2^0) \equiv \hat{w}^*_{\bar{a}}\Phi_a = \epsilon_{\bar{b}\bar{a}}\hat{v}_b\Phi_a. \end{aligned} \quad (9)$$

The transformation between the generic basis and the Higgs basis, $H_a = \hat{U}_{a\bar{b}}\Phi_b$, is given by the following flavor-SU(2) matrix:

$$\hat{U} = \begin{pmatrix} \hat{v}^*_1 & \hat{v}^*_2 \\ \hat{w}^*_1 & \hat{w}^*_2 \end{pmatrix} = \begin{pmatrix} \hat{v}^*_1 & \hat{v}^*_2 \\ -\hat{v}_2 & \hat{v}_1 \end{pmatrix}. \quad (10)$$

This defines a particular Higgs basis.

Inverting Eq. (9) yields:

$$\Phi_a = H_1\hat{v}_a + H_2\hat{w}_a = H_1\hat{v}_a + H_2\hat{v}^*_{\bar{b}}\epsilon_{ba}. \quad (11)$$

The definitions of H_1 and H_2 imply that

$$\langle H_1^0 \rangle = \frac{v}{\sqrt{2}}, \qquad \langle H_2^0 \rangle = 0, \quad (12)$$

where we have used Eq. (6) and the fact that $\hat{v}^*_{\bar{a}}\hat{v}_a = 1$.

The Higgs basis is not unique. Suppose one begins in a generic $\Phi_1' - \Phi_2'$ basis, where $\Phi_a' = V_{a\bar{b}}\Phi_b$ and $\det V \equiv e^{i\chi} \neq 1$. If we now define:

$$H_1' \equiv \hat{v}^*_{\bar{a}}\Phi_a', \qquad H_2' \equiv \hat{w}^*_{\bar{a}}\Phi_a', \quad (13)$$

then

$$H_1' = H_1, \qquad H_2' = (\det V)H_2 = e^{i\chi}H_2. \quad (14)$$

That is, H_1 is an invariant field, whereas H_2 is pseudoinvariant with respect to arbitrary U(2) transformations. In particular, the unitary matrix

$$U_D \equiv \begin{pmatrix} 1 & 0 \\ 0 & e^{i\chi} \end{pmatrix} \quad (15)$$

transforms from the unprimed Higgs basis to the primed Higgs basis. The phase angle χ parameterizes the class of Higgs bases. From the definition of H_2 given in Eq. (9), this phase freedom can be attributed to the choice of an overall phase in the definition of $\hat{w}$ as discussed in Sec. II. This phase freedom will be reflected by the appearance of pseudoinvariants in the study of the Higgs basis. However, pseudoinvariants are useful in that they can be combined to create true invariants, which are candidates for observable quantities.

It is now a simple matter to insert Eq. (11) into Eq. (2) to obtain:

$$\begin{aligned} \mathcal{V} = {} & Y_1H_1^\dagger H_1 + Y_2H_2^\dagger H_2 + [Y_3H_1^\dagger H_2 + \text{H.c.}] \\ & + \frac{1}{2}Z_1(H_1^\dagger H_1)^2 + \frac{1}{2}Z_2(H_2^\dagger H_2)^2 \\ & + Z_3(H_1^\dagger H_1)(H_2^\dagger H_2) + Z_4(H_1^\dagger H_2)(H_2^\dagger H_1) \\ & + \left\{\frac{1}{2}Z_5(H_1^\dagger H_2)^2 + [Z_6(H_1^\dagger H_1) \right. \\ & \left. + Z_7(H_2^\dagger H_2)]H_1^\dagger H_2 + \text{H.c.}\right\}, \end{aligned} \quad (16)$$

where Y_1, Y_2, and $Z_{1,2,3,4}$ are U(2)-invariant quantities and Y_3 and $Z_{5,6,7}$ are pseudoinvariants. The explicit forms for the Higgs basis coefficients have been given in Ref. [17]. The invariant coefficients are conveniently expressed in terms of the second-ranked tensors $V_{a\bar{b}}$ and $W_{a\bar{b}}$ introduced in Sec. II:

$$\begin{aligned} Y_1 &\equiv \text{Tr}(YV), & Y_2 &\equiv \text{Tr}(YW), \\ Z_1 &\equiv Z_{a\bar{b}c\bar{d}}V_{b\bar{a}}V_{d\bar{c}}, & Z_2 &\equiv Z_{a\bar{b}c\bar{d}}W_{b\bar{a}}W_{d\bar{c}}, \\ Z_3 &\equiv Z_{a\bar{b}c\bar{d}}V_{b\bar{a}}W_{d\bar{c}}, & Z_4 &\equiv Z_{a\bar{b}c\bar{d}}V_{b\bar{c}}W_{d\bar{a}}, \end{aligned} \quad (17)$$

whereas the pseudoinvariant coefficients are given by

$$\begin{aligned} Y_3 &\equiv Y_{a\bar{b}}\hat{v}^*_{\bar{a}}\hat{w}_b, & Z_5 &\equiv Z_{a\bar{b}c\bar{d}}\hat{v}^*_{\bar{a}}\hat{w}_b\hat{v}^*_{\bar{c}}\hat{w}_d, \\ Z_6 &\equiv Z_{a\bar{b}c\bar{d}}\hat{v}^*_{\bar{a}}\hat{v}_b\hat{v}^*_{\bar{c}}\hat{w}_d, & Z_7 &\equiv Z_{a\bar{b}c\bar{d}}\hat{v}^*_{\bar{a}}\hat{w}_b\hat{w}^*_{\bar{c}}\hat{w}_d. \end{aligned} \quad (18)$$

The invariant coefficients are manifestly real, whereas the pseudoinvariant coefficients are potentially complex.

Using Eq. (8), it follows that under a flavor-U(2) transformation specified by the matrix U, the pseudoinvariants transform as

$$\begin{aligned} &[Y_3, Z_6, Z_7] \longrightarrow (\det U)^{-1}[Y_3, Z_6, Z_7] \\ &\text{and} \quad Z_5 \longrightarrow (\det U)^{-2}Z_5. \end{aligned} \quad (19)$$

One can also deduce Eq. (19) from Eq. (16) by noting that $\mathcal{V}$ and H_1 are invariant whereas H_2 is pseudoinvariant field that is transforms as

$$H_2 \longrightarrow (\det U)H_2. \quad (20)$$

In the class of Higgs bases defined by Eq. (14), $\hat{v} = (1, 0)$ and $\hat{w} = (0, 1)$, which are independent of the

[3]In tensor calculus, analogous quantities are usually referred to as tensor densities or relative tensors [25].

angle χ that distinguishes among different Higgs bases. That is, under the phase transformation specified by Eq. (15), both $\hat{v}$ and $\hat{w}$ are unchanged. Inserting these values of $\hat{v}$ and $\hat{w}$ into Eqs. (17) and (18) yields the coefficients of the Higgs basis scalar potential. For example, the coefficient of $H_1^\dagger H_2$ is given by $Y_{12} = Y_3$ in the unprimed Higgs basis and $Y'_{12} = Y'_3$ in the primed Higgs basis. Using Eq. (19), it follows that $Y'_{12} = Y_{12}e^{-i\chi}$, which is consistent with the matrix transformation law $Y' = U_D Y U_D^\dagger$.

From the four complex pseudoinvariant coefficients, one can form four independent real invariants $|Y_3|$, $|Z_{5,6,7}|$ and three invariant relative phases $\arg Y_3^2 Z_5^*$, $\arg Y_3 Z_6^*$, and $\arg Y_3 Z_7^*$. Including the six invariants of Eq. (17), we have therefore identified 13 independent invariant real degrees of freedom prior to imposing the scalar potential minimum conditions. Equation (4) then imposes three additional conditions on the set of 13 invariants[4]

$$Y_1 = -\tfrac{1}{2}Z_1 v^2, \qquad Y_3 = -\tfrac{1}{2}Z_6 v^2. \tag{21}$$

This leaves 11 independent real degrees of freedom (one of which is the vacuum expectation value $v = 246$ GeV) that specify the 2HDM parameter space.

The doublet of scalar fields in the Higgs basis can be parameterized as follows:

$$H_1 = \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}}(v + \varphi_1^0 + iG^0) \end{pmatrix}, \qquad H_2 = \begin{pmatrix} H^+ \\ \frac{1}{\sqrt{2}}(\varphi_2^0 + ia^0) \end{pmatrix}, \tag{22}$$

and the corresponding hermitian conjugated fields are likewise defined. We identify $G^\pm$ as a charged Goldstone boson pair and G^0 as the CP-odd neutral Goldstone boson.[5] In particular, the identification of $G^0 = \sqrt{2}\,\mathrm{Im}H_1^0$ follows from the fact that we have defined the Higgs basis [see Eqs. (9) and (12)] such that $\langle H_1^0 \rangle$ is real and nonnegative. Of the remaining fields, φ_1^0 is a CP-even neutral scalar field, φ_2^0 and a^0 are states of indefinite CP quantum numbers,[6] and $H^\pm$ is the physical charged Higgs boson pair. If the Higgs sector is CP-violating, then φ_1^0, φ_2^0, and a^0 all mix to produce three physical neutral Higgs mass-eigenstates of indefinite CP quantum numbers.

IV. THE PHYSICAL 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 minimizing the scalar potential and defining shifted scalar fields with zero vacuum expectation values). This procedure is carried out in Appendix B starting from a generic basis. However, there is an advantage in performing the computation in the Higgs basis since the corresponding scalar potential coefficients are invariant or pseudoinvariant quantities [Eqs. (16)–(18)]. This will allow us to identify U(2)-invariants in the Higgs mass diagonalization procedure.

Thus, we proceed by inserting Eq. (11) into Eq. (2) and examining the terms linear and quadratic in the scalar fields. The requirement that the coefficient of the linear term vanishes corresponds to the scalar potential minimum conditions [Eq. (21)]. These conditions are then used in the evaluation of the coefficients of the terms quadratic in the fields. One can easily check that no quadratic terms involving the Goldstone boson fields survive (as expected, since the Goldstone bosons are massless). This confirms our identification of the Goldstone fields in Eq. (22). The charged Higgs boson mass is also easily determined:

$$m_{H^\pm}^2 = Y_2 + \tfrac{1}{2}Z_3 v^2. \tag{23}$$

The three remaining neutral fields mix, and the resulting neutral Higgs squared-mass matrix in the $\varphi_1^0 - \varphi_2^0 - a^0$ basis is

$$\mathcal{M} = v^2 \begin{pmatrix} Z_1 & \mathrm{Re}(Z_6) & -\mathrm{Im}(Z_6) \\ \mathrm{Re}(Z_6) & \frac{1}{2}[Z_3 + Z_4 + \mathrm{Re}(Z_5)] + Y_2/v^2 & -\frac{1}{2}\mathrm{Im}(Z_5) \\ -\mathrm{Im}(Z_6) & -\frac{1}{2}\mathrm{Im}(Z_5) & \frac{1}{2}[Z_3 + Z_4 - \mathrm{Re}(Z_5)] + Y_2/v^2 \end{pmatrix}. \tag{24}$$

Note that $\mathcal{M}$ depends implicitly on the choice of Higgs basis [Eq. (14)] via the χ-dependence of the pseudoinvariants Z_5 and Z_6. Moreover, the real and imaginary parts of these pseudoinvariants mix if χ is changed. Thus, $\mathcal{M}$ does not possess simple transformation properties under arbitrary flavor-U(2) transformations. Nevertheless, we demonstrate below that the eigenvalues and normalized eigenvectors are U(2)-invariant. First, we compute the

[4]The second condition of Eq. (21) is a complex equation that can be rewritten in terms of invariants: $|Y_3| = \frac{1}{2}|Z_6|v^2$ and $Y_3 Z_6^* = -\frac{1}{2}|Z_6|^2 v^2$.

[5]The definite CP property of the neutral Goldstone boson persists even if the Higgs Lagrangian is CP-violating (either explicitly or spontaneously), as shown in Appendix D.

[6]The CP-properties of the neutral scalar fields (in the Higgs basis) can be determined by studying the pattern of gauge boson/scalar boson couplings and the scalar self-couplings in the interaction Lagrangian (see Sec. V). If the scalar potential is CP-conserving, then two orthogonal linear combinations of φ_2^0 and a^0 can be found that are eigenstates of CP. By an appropriate rephasing of H_2 (which corresponds to some particular choice among the possible Higgs bases) such that all the coefficients of the scalar potential in the Higgs basis are real, one can then identify φ_2^0 as a CP-even scalar field and a^0 as a CP-odd scalar field. See Appendix D for further details.

characteristic equation:

$$\det(\mathcal{M} - xI) = -x^3 + \mathrm{Tr}(\mathcal{M})x^2 - \tfrac{1}{2}[(\mathrm{Tr}\mathcal{M})^2 - \mathrm{Tr}(\mathcal{M}^2)]x + \det(\mathcal{M}), \quad (25)$$

where I is the 3×3 identity matrix. [The coefficient of x in Eq. (25) is particular to 3×3 matrices (see Fact 4.9.3 of Ref. [26]).] Explicitly,

$$\begin{aligned}
\mathrm{Tr}(\mathcal{M}) &= 2Y_2 + (Z_1 + Z_3 + Z_4)v^2, \\
\mathrm{Tr}(\mathcal{M}^2) &= Z_1^2 v^4 + \tfrac{1}{2}v^4[(Z_3 + Z_4)^2 + |Z_5|^2 + 4|Z_6|^2] \\
&\quad + 2Y_2[Y_2 + (Z_3 + Z_4)v^2], \\
\det(\mathcal{M}) &= \tfrac{1}{4}\{Z_1 v^6[(Z_3 + Z_4)^2 - |Z_5|^2] \\
&\quad - 2v^4[2Y_2 + (Z_3 + Z_4)v^2]|Z_6|^2 \\
&\quad + 4Y_2 Z_1 v^2[Y_2 + (Z_3 + Z_4)v^2] + 2v^6 \,\mathrm{Re}(Z_5^* Z_6^2)\}.
\end{aligned} \quad (26)$$

Clearly, all the coefficients of the characteristic polynomial are U(2)-invariant. Since the roots of this polynomial are the squared-masses of the physical Higgs bosons, it follows that the physical Higgs masses are basis-independent as required. Since $\mathcal{M}$ is a real symmetric matrix, the eigenvalues of $\mathcal{M}$ are real. However, if any of these eigenvalues are negative, then the extremal solution of Eq. (4) with $v \neq 0$ is *not* a minimum of the scalar potential. The requirements that $m_{H^\pm}^2 > 0$ [Eq. (23)] and the positivity of the squared-mass eigenvalues of $\mathcal{M}$ provide basis-independent conditions for the desired spontaneous symmetry-breaking pattern specified by Eq. (3).

The real symmetric squared-mass matrix $\mathcal{M}$ can be diagonalized by an orthogonal transformation

$$R\mathcal{M}R^T = \mathcal{M}_D \equiv \mathrm{diag}(m_1^2, m_2^2, m_3^2), \quad (27)$$

where $RR^T = I$ and the m_k^2 are the eigenvalues of $\mathcal{M}$ [i.e., the roots of Eq. (25)]. A convenient form for R is

$$\begin{aligned}
R &= R_{12}R_{13}R_{23} \\
&= \begin{pmatrix} c_{12} & -s_{12} & 0 \\ s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} c_{13} & 0 & -s_{13} \\ 0 & 1 & 0 \\ s_{13} & 0 & c_{13} \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & -s_{23} \\ 0 & s_{23} & c_{23} \end{pmatrix} \\
&= \begin{pmatrix} c_{13}c_{12} & -c_{23}s_{12} - c_{12}s_{13}s_{23} & -c_{12}c_{23}s_{13} + s_{12}s_{23} \\ c_{13}s_{12} & c_{12}c_{23} - s_{12}s_{13}s_{23} & -c_{23}s_{12}s_{13} - c_{12}s_{23} \\ s_{13} & c_{13}s_{23} & c_{13}c_{23} \end{pmatrix},
\end{aligned} \quad (28)$$

where $c_{ij} \equiv \cos\theta_{ij}$ and $s_{ij} \equiv \sin\theta_{ij}$. Note that $\det R = 1$, although we could have chosen an orthogonal matrix with determinant equal to -1 by choosing $-R$ in place of R. In addition, if we take the range of the angles to be $-\pi \leq \theta_{12}, \theta_{23} < \pi$, and $|\theta_{13}| \leq \pi/2$, then we cover the complete parameter space of SO(3) matrices (see p. 11 of Ref. [24]). That is, we work in a convention where $c_{13} \geq 0$. However, this parameter space includes points that simply correspond to the redefinition of two of the Higgs mass-eigenstate fields by their negatives. Thus, we may reduce the parameter space further and define all Higgs mixing angles modulo π. We shall verify this assertion at the end of this section.

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

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R\begin{pmatrix} \varphi_1^0 \\ \varphi_2^0 \\ a^0 \end{pmatrix}. \quad (29)$$

It is often convenient to choose a convention for the mass ordering of the h_k such that $m_1 \leq m_2 \leq m_3$.

Since the mass-eigenstates h_k do not depend on the initial basis choice, they must be U(2)-invariant fields. In order to present a formal proof of this assertion, we need to determine the transformation properties of the elements of R under an arbitrary U(2) transformation. In principle, these can be determined from Eq. (27), using the fact that the m_k^2 are invariant quantities. However, the form of $\mathcal{M}$ is not especially convenient for this purpose as noted below Eq. (24). This can be ameliorated by introducing the unitary matrix:

$$W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & -i/\sqrt{2} & i/\sqrt{2} \end{pmatrix}, \quad (30)$$

and rewriting Eq. (27) as

$$(RW)(W^\dagger \mathcal{M} W)(RW)^\dagger = \mathcal{M}_D = \mathrm{diag}(m_1^2, m_2^2, m_3^2). \quad (31)$$

A straightforward calculation yields:

$$W^\dagger \mathcal{M} W = v^2 \begin{pmatrix} Z_1 & \frac{1}{\sqrt{2}}Z_6 & \frac{1}{\sqrt{2}}Z_6^* \\ \frac{1}{\sqrt{2}}Z_6^* & \frac{1}{2}(Z_3 + Z_4) + Y_2/v^2 & \frac{1}{2}Z_5^* \\ \frac{1}{\sqrt{2}}Z_6 & \frac{1}{2}Z_5 & \frac{1}{2}(Z_3 + Z_4) + Y_2/v^2 \end{pmatrix}, \quad (32)$$

$$RW = \begin{pmatrix} q_{11} & \frac{1}{\sqrt{2}}q_{12}^* e^{i\theta_{23}} & \frac{1}{\sqrt{2}}q_{12}e^{-i\theta_{23}} \\ q_{21} & \frac{1}{\sqrt{2}}q_{22}^* e^{i\theta_{23}} & \frac{1}{\sqrt{2}}q_{22}e^{-i\theta_{23}} \\ q_{31} & \frac{1}{\sqrt{2}}q_{32}^* e^{i\theta_{23}} & \frac{1}{\sqrt{2}}q_{32}e^{-i\theta_{23}} \end{pmatrix}, \quad (33)$$

where

$$\begin{aligned} q_{11} &= c_{13}c_{12}, & q_{12} &= -s_{12} - ic_{12}s_{13}, \\ q_{21} &= c_{13}s_{12}, & q_{22} &= c_{12} - is_{12}s_{13}, \\ q_{31} &= s_{13}, & q_{32} &= ic_{13}. \end{aligned} \tag{34}$$

The matrix RW defined in Eq. (33) is unitary and satisfies $\det RW = i$. Evaluating this determinant yields:

$$\frac{1}{2}\sum_{j,k,\ell=1}^{3} \epsilon_{jk\ell} q_{j1}\,\mathrm{Im}(q_{k2}^* q_{\ell 2}) = 1, \tag{35}$$

while unitarity implies:

$$\mathrm{Re}\,(q_{k1}q_{\ell 1}^* + q_{k2}q_{\ell 2}^*) = \delta_{k\ell}, \tag{36}$$

$$\begin{aligned} \sum_{k=1}^{3} |q_{k1}|^2 &= \frac{1}{2}\sum_{k=1}^{3}|q_{k2}|^2 = 1, \\ \sum_{k=1}^{3} q_{k2}^2 &= \sum_{k=1}^{3} q_{k1}q_{k2} = 0. \end{aligned} \tag{37}$$

These results can be used to prove the identity [27]:

$$q_{j1} = \frac{1}{2}\sum_{k,\ell=1}^{3} \epsilon_{jk\ell}\,\mathrm{Im}(q_{k2}^* q_{\ell 2}). \tag{38}$$

Since the matrix elements of $W^\dagger \mathcal{M} W$ only involve invariants and pseudoinvariants, we may use Eq. (31) to determine the flavor-U(2) transformation properties of $q_{k\ell}$ and $e^{i\theta_{23}}$. The resulting transformation laws are

$$q_{k\ell} \rightarrow q_{k\ell} \quad \text{and} \quad e^{i\theta_{23}} \rightarrow (\det U)^{-1} e^{i\theta_{23}}, \tag{39}$$

under a U(2) transformation U. That is, the $q_{k\ell}$ are invariants, or equivalently θ_{12} and θ_{13} (modulo π) are U(2)-invariant angles, whereas $e^{i\theta_{23}}$ is a pseudoinvariant. Equation (39) is critical for the rest of the paper. Finally, to show that the Higgs mass-eigenstates are invariant fields, we rewrite Eq. (29) as

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = RW \begin{pmatrix} \sqrt{2}\,\mathrm{Re}H_1^0 - v \\ H_2^0 \\ H_2^{0\dagger} \end{pmatrix}. \tag{40}$$

Since the $q_{k\ell}$, H_1, and the product $e^{i\theta_{23}}H_2$ are U(2)-invariant quantities, it follows that the h_k are invariant fields.

The transformation laws given in Eqs. (19) and (39) imply that the quantities $Z_5 e^{-2i\theta_{23}}$, $Z_6 e^{-i\theta_{23}}$, and $Z_7 e^{-i\theta_{23}}$ are U(2)-invariant. These combinations will appear in the physical Higgs boson self-couplings of Sec. V and in the expressions for the invariant mixing angles given in Appendix C. With this in mind, it is useful to rewrite the neutral Higgs mass diagonalization equation [Eq. (27)] as follows. With $R \equiv R_{12}R_{13}R_{23}$ given by Eq. (28), we define

$$\tilde{\mathcal{M}} \equiv R_{23}\mathcal{M}R_{23}^T = v^2 \begin{pmatrix} Z_1 & \mathrm{Re}(Z_6 e^{-i\theta_{23}}) & -\mathrm{Im}(Z_6 e^{-i\theta_{23}}) \\ \mathrm{Re}(Z_6 e^{-i\theta_{23}}) & \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) + A^2/v^2 & -\frac{1}{2}\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) \\ -\mathrm{Im}(Z_6 e^{-i\theta_{23}}) & -\frac{1}{2}\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) & A^2/v^2 \end{pmatrix}. \tag{41}$$

where A^2 is defined by

$$A^2 \equiv Y_2 + \tfrac{1}{2}[Z_3 + Z_4 - \mathrm{Re}(Z_5 e^{-2i\theta_{23}})]v^2. \tag{42}$$

The diagonal neutral Higgs squared-mass matrix is then given by

$$\tilde{R}\,\tilde{\mathcal{M}}\,\tilde{R}^T = \mathcal{M}_D = \mathrm{diag}(m_1^2, m_2^2, m_3^2), \tag{43}$$

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

$$\tilde{R} = \begin{pmatrix} c_{12}c_{13} & -s_{12} & -c_{12}s_{13} \\ c_{13}s_{12} & c_{12} & -s_{12}s_{13} \\ s_{13} & 0 & c_{13} \end{pmatrix}. \tag{44}$$

Equations (41)–(44) provide a manifestly U(2)-invariant squared-mass matrix diagonalization, since the elements of $\tilde{R}$ and $\tilde{\mathcal{M}}$ are invariant quantities.

In this section, all computations were carried out by first transforming to the Higgs basis. The advantage of this procedure is that one can readily identify the relevant invariant and pseudoinvariant quantities involved in the determination of the Higgs mass-eigenstates. We may now combine Eqs. (9) and (40) to obtain explicit expressions for the Higgs mass-eigenstate fields h_k in terms of the scalar fields in the generic basis Φ_a. Since these expressions do not depend on the Higgs basis, one could have obtained the results for the Higgs mass-eigenstates directly without reference to Higgs basis quantities. In Appendix B, we present a derivation starting from the generic basis, which produces the following expressions for the Higgs mass-eigenstates (and the Goldstone boson) in terms of the generic-basis fields:

$$\begin{aligned} h_k = \frac{1}{\sqrt{2}}[&\bar{\Phi}_{\bar{a}}^{0\dagger}(q_{k1}\hat{v}_a + q_{k2}\hat{w}_a e^{-i\theta_{23}}) \\ &+ (q_{k1}^*\hat{v}_{\bar{a}}^* + q_{k2}^*\hat{w}_{\bar{a}}^* e^{i\theta_{23}})\bar{\Phi}_a^0], \end{aligned} \tag{45}$$

for $k = 1, \ldots, 4$, where $h_4 = G^0$. 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 defined for $k = 1, 2, 3$ and $\ell = 1, 2$ by Eq. (34). To account for the Goldstone boson ($k = 4$) we have also introduced: $q_{41} = i$ and $q_{42} = 0$. For the reader's convenience, the explicit forms for the $q_{k\ell}$ are displayed in Table I. Since the $q_{k\ell}$ are U(2)-invariant and $\hat{w}_a e^{-i\theta_{23}}$ is a *proper* vector under U(2) transformations, it follows that Eq. (45) provides a U(2)-invariant expression for the Higgs mass-eigenstates.

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

k	q_{k1}	q_{k2}
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}
4	i	0

It is now a simple matter to invert Eq. (45) to obtain

$$\Phi_a = \begin{pmatrix} G^+ \hat{v}_a + H^+ \hat{w}_a \\ \frac{v}{\sqrt{2}}\hat{v}_a + \frac{1}{\sqrt{2}}\sum_{k=1}^{4}(q_{k1}\hat{v}_a + q_{k2}e^{-i\theta_{23}}\hat{w}_a)h_k \end{pmatrix}, \quad (46)$$

where $h_4 \equiv G^0$. The form of the charged upper component of Φ_a is a consequence of Eq. (11). The U(2)-covariant expression for Φ_a in terms of the Higgs mass-eigenstate scalar fields given by Eq. (46) is one of the central results of this paper. In Secs. V and VI, we shall employ this result for Φ_a in the computation of the Higgs couplings of the 2HDM.

Finally, we return to the question of the domains of the angles θ_{ij}. We assume that $Z_6 \equiv |Z_6|e^{i\theta_6} \neq 0$ (the special case of $Z_6 = 0$ is treated at the end of Appendix C). Since $e^{-i\theta_{23}}$ is a pseudoinvariant, we prefer to deal with the invariant angle ϕ:

$$\phi \equiv \theta_6 - \theta_{23}, \quad \text{where} \quad \theta_6 \equiv \arg Z_6. \quad (47)$$

As shown in Appendix C, the invariant angles θ_{12}, θ_{13}, and ϕ are determined modulo π in terms of invariant combinations of the scalar potential parameters. This domain is smaller than the one defined by $-\pi \leq \theta_{12}$, $\theta_{23} < \pi$ and $|\theta_{13}| \leq \pi/2$, which covers the parameter space of SO(3) matrices. Since the U(2)-invariant mass-eigenstate fields h_k are real, one can always choose to redefine any one of the h_k by its negative. Redefining two of the three Higgs fields h_1, h_2 and h_3 by their negatives[7] is equivalent to multiplying two of the rows of R by -1. In particular,

$$\theta_{12} \to \theta_{12} \pm \pi \Rightarrow h_1 \to -h_1 \quad \text{and} \quad h_2 \to -h_2, \quad (48)$$

$$\phi \to \phi \pm \pi, \quad \theta_{13} \to -\theta_{13}, \quad \theta_{12} \to \pm\pi - \theta_{12} \Rightarrow h_1 \to -h_1 \quad \text{and} \quad h_3 \to -h_3, \quad (49)$$

$$\theta_{13} \to \theta_{13} \pm \pi, \quad \theta_{12} \to -\theta_{12} \Rightarrow h_1 \to -h_1 \quad \text{and} \quad h_3 \to -h_3, \quad (50)$$

$$\phi \to \phi \pm \pi, \quad \theta_{13} \to -\theta_{13}, \quad \theta_{12} \to -\theta_{12} \Rightarrow h_2 \to -h_2 \quad \text{and} \quad h_3 \to -h_3, \quad (51)$$

$$\theta_{13} \to \theta_{13} \pm \pi, \quad \theta_{12} \to \pm\pi - \theta_{12} \Rightarrow h_2 \to -h_2 \quad \text{and} \quad h_3 \to -h_3. \quad (52)$$

This means that if we adopt a convention in which c_{12}, c_{13}, and $\sin\phi$ are non-negative, with the angles defined modulo π, then the sign of the Higgs mass-eigenstate fields will be fixed.

Given a choice of the overall sign conventions of the neutral Higgs fields, the number of solutions for the invariant angles θ_{12}, θ_{13}, and ϕ modulo π are in one-to-one correspondence with the possible mass orderings of the m_k (except at certain singular points of the parameter space[8]). For example, note that

$$\theta_{12} \to \theta_{12} \pm \pi/2 \Rightarrow h_1 \to \mp h_2 \quad \text{and} \quad h_2 \to \pm h_1. \quad (53)$$

That is, two solutions for θ_{12} exist modulo π. If $m_1 < m_2$, then Eq. (C24) implies that the solutions for θ_{12} and ϕ are correlated such that $s_{12}\cos\phi \geq 0$, and (for fixed ϕ) only one θ_{12} solution modulo π survives. The corresponding effects on the invariant angles that result from swapping other pairs of neutral Higgs fields are highly nonlinear and cannot be simply exhibited in closed form. Nevertheless, we can use the results of Appendix C to conclude that for $m_{1,2} < m_3$ (in a convention where $\sin\phi \geq 0$), Eq. (C22) yields $s_{13} \leq 0$, and for $m_1 < m_2 < m_3$, Eq. (C20) implies that $\sin 2\theta_{56}\cos\phi \geq 0$, where $\theta_{56} \equiv -\frac{1}{2}\arg(Z_5^* Z_6^2)$.

The sign of the neutral Goldstone field is conventional, but is not affected by the choice of Higgs mixing angles. Finally, we note that the charged fields $G^\pm$ and $H^\pm$ are complex. Equation (46) implies that $G^\pm$ is an invariant field and $H^\pm$ is a pseudoinvariant field that transforms as

$$H^\pm \to (\det U)^{\pm 1} H^\pm \quad (54)$$

with respect to U(2) transformations. That is, once the Higgs Lagrangian is written in terms the Higgs mass-eigenstates and the Goldstone bosons, one is still free to rephase the charged fields. By convention, we shall fix this phase according to Eq. (46).

V. HIGGS COUPLINGS TO BOSONS

We begin by computing the Higgs self-couplings in terms of U(2)-invariant quantities. First, we use Eq. (46) to obtain:

[7]In order to have an odd number of Higgs mass-eigenstates redefined by their negatives, one would have to employ an orthogonal Higgs mixing matrix with $\det R = -1$.

[8]At singular points of the parameter space corresponding to two (or three) mass-degenerate neutral Higgs bosons, some (or all) of the invariant Higgs mixing angles are indeterminate. An indeterminate invariant angle also arises in the case of $Z_6 = 0$ and $c_{13} = 0$ as explained at the end of Appendix C.

$$\begin{aligned}\Phi_{\bar{a}}^\dagger\Phi_b &= \tfrac{1}{2}v^2V_{b\bar{a}} + vh_k[V_{b\bar{a}}\,\mathrm{Re}q_{k1} + \tfrac{1}{2}(\hat{v}_b\hat{w}_{\bar{a}}^*q_{k2}^*e^{i\theta_{23}} \\ &\quad + \hat{v}_{\bar{a}}^*\hat{w}_bq_{k2}e^{-i\theta_{23}})] + \tfrac{1}{2}h_jh_k[V_{b\bar{a}}\,\mathrm{Re}(q_{j1}^*q_{k1}) \\ &\quad + W_{b\bar{a}}\,\mathrm{Re}(q_{j2}^*q_{k2}) + \hat{v}_b\hat{w}_{\bar{a}}^*q_{j_2}^*q_{k1}e^{i\theta_{23}} \\ &\quad + \hat{v}_{\bar{a}}^*\hat{w}_bq_{j1}^*q_{k2}e^{-i\theta_{23}}] + G^+G^-V_{b\bar{a}} + H^+H^-W_{b\bar{a}} \\ &\quad + G^-H^+\hat{v}_{\bar{a}}^*\hat{w}_b + G^+H^-\hat{w}_{\bar{a}}^*\hat{v}_b, \end{aligned} \tag{55}$$

where repeated indices are summed over and $j, k = 1, \ldots, 4$. We then insert Eq. (55) into Eq. (2), and expand out the resulting expression. We shall write:

$$\mathcal{V} = \mathcal{V}_0 + \mathcal{V}_2 + \mathcal{V}_3 + \mathcal{V}_4, \tag{56}$$

where the subscript indicates the overall degree of the fields that appears in the polynomial expression. $\mathcal{V}_0$ is a constant of no significance and $\mathcal{V}_1 = 0$ by the scalar potential minimum condition. $\mathcal{V}_2$ is obtained in Appendix C. In this section, we focus on the cubic Higgs self-couplings that reside in $\mathcal{V}_3$ and the quartic Higgs self-couplings that reside in $\mathcal{V}_4$.

Using Eqs. (17) and (18), one can express $\mathcal{V}_3$ and $\mathcal{V}_4$ in terms of the invariants (Y_1, Y_2, and $Z_{1,2,3,4}$) and pseudoinvariants (Y_3, $Z_{5,6,7}$). In the resulting expressions, we have eliminated Y_1 and Y_3 by the scalar potential minimum conditions [Eq. (21)]. The cubic Higgs couplings are governed by the following terms of the scalar potential:

$$\begin{aligned}\mathcal{V}_3 &= \tfrac{1}{2}vh_jh_kh_\ell[q_{j1}q_{k1}^*\,\mathrm{Re}(q_{\ell1})Z_1 + q_{j2}q_{k2}^*\,\mathrm{Re}(q_{\ell1})(Z_3+Z_4) + \mathrm{Re}(q_{j1}^*q_{k2}q_{\ell2}Z_5e^{-2i\theta_{23}}) + \mathrm{Re}([2q_{j1}+q_{j1}^*]q_{k1}^*q_{\ell2}Z_6e^{-i\theta_{23}}) \\ &\quad + \mathrm{Re}(q_{j2}^*q_{k2}q_{\ell2}Z_7e^{-i\theta_{23}})] + vh_kG^+G^-[\mathrm{Re}(q_{k1})Z_1 + \mathrm{Re}(q_{k2}e^{-i\theta_{23}}Z_6)] + vh_kH^+H^-[\mathrm{Re}(q_{k1})Z_3 + \mathrm{Re}(q_{k2}e^{-i\theta_{23}}Z_7)] \\ &\quad + \tfrac{1}{2}vh_k\{G^-H^+e^{i\theta_{23}}[q_{k2}^*Z_4 + q_{k2}e^{-2i\theta_{23}}Z_5 + 2\,\mathrm{Re}(q_{k1})Z_6e^{-i\theta_{23}}] + \mathrm{H.c.}\},\end{aligned} \tag{57}$$

where there is an implicit sum over the repeated indices[9] $j, k, \ell = 1, 2, 3, 4$. Since the neutral Goldstone boson field is denoted by $h_4 \equiv G^0$, we can extract the cubic couplings of G^0 by using $q_{41} = i$ and $q_{42} = 0$. The only cubic Higgs-G^0 couplings that survive are

$$\mathcal{V}_{3G} = \frac{1}{2}v\sum_{k=1}^{3}\sum_{\ell=1}^{3}G^0h_kh_\ell[\mathrm{Im}(q_{k2}q_{\ell2}Z_5e^{-2i\theta_{23}}) + 2q_{k1}\,\mathrm{Im}(q_{\ell2}Z_6e^{-i\theta_{23}})] + \frac{1}{2}v\sum_{\ell=1}^{3}G^0G^0h_\ell[q_{\ell1}Z_1 + \mathrm{Re}(q_{\ell2}Z_6e^{-i\theta_{23}})], \tag{58}$$

where we have used the fact that q_{j1} is real for $j = 1, 2, 3$.

At the end of the Sec. IV, we noted that H^+ is a pseudoinvariant field. However $e^{i\theta_{23}}H^+$ is a $U(2)$-invariant field [see Eqs. (39) and (54)], and it is precisely this combination that shows up in Eq. (57). Moreover, as shown in Sec. IV, the $q_{k\ell}$ and the quantities $Z_5e^{-2i\theta_{23}}$, $Z_6e^{-i\theta_{23}}$ and $Z_7e^{-i\theta_{23}}$ are also invariant with respect to flavor-U(2) transformations. Thus, we conclude that Eq. (57) is U(2)-invariant as required.

The quartic Higgs couplings are governed by the following terms of the scalar potential:

$$\begin{aligned}\mathcal{V}_4 &= \tfrac{1}{8}h_jh_kh_lh_m[q_{j1}q_{k1}q_{\ell1}^*q_{m1}^*Z_1 + q_{j2}q_{k2}q_{\ell2}^*q_{m2}^*Z_2 + 2q_{j1}q_{k1}^*q_{\ell2}q_{m2}^*(Z_3+Z_4) + 2\,\mathrm{Re}(q_{j1}^*q_{k1}^*q_{\ell2}q_{m2}Z_5e^{-2i\theta_{23}}) \\ &\quad + 4\,\mathrm{Re}(q_{j1}q_{k1}^*q_{\ell1}^*q_{m2}Z_6e^{-i\theta_{23}}) + 4\,\mathrm{Re}(q_{j1}^*q_{k2}q_{\ell2}q_{m2}^*Z_7e^{-i\theta_{23}})] + \tfrac{1}{2}h_jh_kG^+G^-[q_{j1}q_{k1}^*Z_1 + q_{j2}q_{k2}^*Z_3 \\ &\quad + 2\,\mathrm{Re}(q_{j1}q_{k2}Z_6e^{-i\theta_{23}})] + \tfrac{1}{2}h_jh_kH^+H^-[q_{j2}q_{k2}^*Z_2 + q_{j1}q_{k1}^*Z_3 + 2\,\mathrm{Re}(q_{j1}q_{k2}Z_7e^{-i\theta_{23}})] \\ &\quad + \tfrac{1}{2}h_jh_k\{G^-H^+e^{i\theta_{23}}[q_{j1}q_{k2}^*Z_4 + q_{j1}^*q_{k2}Z_5e^{-2i\theta_{23}} + q_{j1}q_{k1}^*Z_6e^{-i\theta_{23}} + q_{j2}q_{k2}^*Z_7e^{-i\theta_{23}}] + \mathrm{H.c.}\} \\ &\quad + \tfrac{1}{2}Z_1G^+G^-G^+G^- + \tfrac{1}{2}Z_2H^+H^-H^+H^- + (Z_3+Z_4)G^+G^-H^+H^- + \tfrac{1}{2}Z_5H^+H^+G^-G^- + \tfrac{1}{2}Z_5^*H^-H^-G^+G^+ \\ &\quad + G^+G^-(Z_6H^+G^- + Z_6^*H^-G^+) + H^+H^-(Z_7H^+G^- + Z_7^*H^-G^+),\end{aligned} \tag{59}$$

where there is an implicit sum over the repeated indices $j, k, \ell, m = 1, 2, 3, 4$. One can check the U(2)-invariance of $\mathcal{V}_4$ by noting that $Z_5H^+H^+$, Z_6H^+, and Z_7H^+ are U(2)-invariant combinations.[10] It is again straightforward to isolate the quartic couplings of the neutral Goldstone boson ($h_4 \equiv G^0$):

[9]Note that the sum over repeated indices can be rewritten by appropriately symmetrizing the relevant coefficients. For example, $\sum_{jk\ell}g_{jk\ell}h_jh_kh_\ell = \sum_{j\le k\le l}h_jh_kh_\ell[g_{jk\ell} + \mathrm{perm}]$, where "perm" is an instruction to add additional terms (as needed) such that the indices j, k, and ℓ appear in all possible *distinct* permutations.

[10]It is instructive to write, e.g., $Z_6H^+ = (Z_6e^{-i\theta_{23}})(H^+e^{i\theta_{23}})$, etc. to exhibit the well-known U(2)-invariant combinations.

$$\begin{aligned}\mathcal{V}_{4G} = {} & \tfrac{1}{8}q_{11}^4 Z_1 G^0G^0G^0G^0 + \tfrac{1}{2}\mathrm{Im}(q_{m2}Z_6 e^{-i\theta_{23}})G^0G^0G^0h_m + \tfrac{1}{4}G^0G^0h_\ell h_m[q_{\ell 1}q_{m1}Z_1 + q_{\ell 2}q_{m2}^*(Z_3+Z_4) \\ & - \mathrm{Re}(q_{\ell 2}q_{m2}Z_5 e^{-2i\theta_{23}}) + 2q_{\ell 1}\,\mathrm{Re}(q_{m2}Z_6 e^{-i\theta_{23}})] + \tfrac{1}{2}G^0h_k h_\ell h_m[q_{k1}\,\mathrm{Re}(q_{\ell 2}q_{m2}Z_5 e^{-2i\theta_{23}}) \\ & + q_{k1}q_{\ell 1}\,\mathrm{Re}(q_{m2}Z_6 e^{-i\theta_{23}}) + \mathrm{Re}(q_{k2}q_{\ell 2}q_{m2}^*Z_7 e^{-i\theta_{23}})] - \mathrm{Im}(q_{m2}Z_6 e^{-i\theta_{23}})G^+G^-G^0h_m \\ & - \mathrm{Im}(q_{m2}Z_7 e^{-i\theta_{23}})H^+H^-G^0h_m + \tfrac{1}{2}iG^0h_m\{G^-H^+e^{i\theta_{23}}[q_{m2}^*Z_4 - q_{m2}Z_5 e^{-2i\theta_{23}}] + \mathrm{H.c.}\} \\ & + \tfrac{1}{2}Z_1G^0G^0G^+G^- + \tfrac{1}{2}Z_3G^0G^0H^+H^- + \tfrac{1}{2}Z_6G^0G^0G^-H^+ + \tfrac{1}{2}Z_6^*G^0G^0G^+H^-, \end{aligned} \tag{60}$$

where the repeated indices $k, \ell, m = 1, 2, 3$ are summed over.

The Feynman rules are obtained by multiplying the relevant terms of the scalar potential by $-iS$, where the symmetry factor $S = \prod_i n_i!$ for an interaction term that possesses n_i identical particles of type i. Explicit forms for the $q_{k\ell}$ in terms of the invariant mixing angles θ_{12} and θ_{13} are displayed in Table I. For example, the Feynman rule for the cubic self-coupling of the lightest neutral Higgs boson is given by $ig(h_1h_1h_1)$ where

$$\begin{aligned} g(h_1h_1h_1) = {} & -3v[Z_1c_{12}^3c_{13}^3 + (Z_3+Z_4)c_{12}c_{13}|s_{123}|^2 \\ & + c_{12}c_{13}\,\mathrm{Re}(s_{123}^2Z_5e^{-2i\theta_{23}}) \\ & - 3c_{12}^2c_{13}^2\,\mathrm{Re}(s_{123}Z_6e^{-i\theta_{23}}) \\ & - |s_{123}|^2\mathrm{Re}(s_{123}Z_7e^{-i\theta_{23}})], \end{aligned} \tag{61}$$

where $s_{123} \equiv s_{12} + ic_{12}s_{13}$. Similarly, the Feynman rule for the quartic self-coupling of the lightest neutral Higgs boson is given by $ig(h_1h_1h_1h_1)$ where

$$\begin{aligned} g(h_1h_1h_1h_1) = {} & -3[Z_1c_{12}^4c_{13}^4 + Z_2|s_{123}|^4 \\ & + 2(Z_3+Z_4)c_{12}^2c_{13}^2|s_{123}|^2 \\ & + 2c_{12}^2c_{13}^2\,\mathrm{Re}(s_{123}^2Z_5e^{-2i\theta_{23}}) \\ & - 4c_{12}^3c_{13}^3\,\mathrm{Re}(s_{123}Z_6e^{-i\theta_{23}}) \\ & - 4c_{12}c_{13}|s_{123}|^2\mathrm{Re}(s_{123}Z_7e^{-i\theta_{23}})]. \end{aligned} \tag{62}$$

We turn next to the coupling of the Higgs bosons to the gauge bosons. These arise from the Higgs boson kinetic energy terms when the partial derivatives are replaced by the gauge covariant derivatives: $\mathcal{L}_{\mathrm{KE}} = D^\mu\Phi_{\bar a}^\dagger D_\mu\Phi_a$. In the $\mathrm{SU(2)_L}\times\mathrm{U(1)}$ electroweak gauge theory,

$$D_\mu\Phi_a = \begin{pmatrix} \partial_\mu\Phi_a^+ + \left[\frac{ig}{c_W}\left(\frac{1}{2}-s_W^2\right)Z_\mu + ieA_\mu\right]\Phi_a^+ + \frac{ig}{\sqrt{2}}W_\mu^+\Phi_a^0 \\ \partial_\mu\Phi_a^0 - \frac{ig}{2c_W}Z_\mu\Phi_a^0 + \frac{ig}{\sqrt{2}}W_\mu^-\Phi_a^+ \end{pmatrix}, \tag{63}$$

where $s_W \equiv \sin\theta_W$ and $c_W \equiv \cos\theta_W$. Inserting Eq. (63) into $\mathcal{L}_{\mathrm{KE}}$ yields the Higgs boson-gauge boson interactions in the generic basis. Finally, we use Eq. (46) to obtain the interaction Lagrangian of the gauge bosons with the physical Higgs boson mass-eigenstates. The resulting interaction terms are

$$\mathcal{L}_{VVH} = \left(gm_WW_\mu^+W^{\mu-} + \frac{g}{2c_W}m_ZZ_\mu Z^\mu\right)\mathrm{Re}(q_{k1})h_k + em_WA^\mu(W_\mu^+G^- + W_\mu^-G^+) - gm_Zs_W^2Z^\mu(W_\mu^+G^- + W_\mu^-G^+), \tag{64}$$

$$\begin{aligned} \mathcal{L}_{VVHH} = {} & \left[\frac{1}{4}g^2W_\mu^+W^{\mu-} + \frac{g^2}{8c_W^2}Z_\mu Z^\mu\right]\mathrm{Re}(q_{j1}^*q_{k1} + q_{j2}^*q_{k2})h_jh_k \\ & + \left[e^2A_\mu A^\mu + \frac{g^2}{c_W^2}\left(\frac{1}{2}-s_W^2\right)^2Z_\mu Z^\mu + \frac{2ge}{c_W}\left(\frac{1}{2}-s_W^2\right)A_\mu Z^\mu\right](G^+G^- + H^+H^-) \\ & + \left\{\left(\frac{1}{2}egA^\mu W_\mu^+ - \frac{g^2s_W^2}{2c_W}Z^\mu W_\mu^+\right)(q_{k1}G^- + q_{k2}e^{-i\theta_{23}}H^-)h_k + \mathrm{H.c.}\right\}, \end{aligned} \tag{65}$$

and

$$\begin{aligned} \mathcal{L}_{VHH} = {} & \frac{g}{4c_W}\,\mathrm{Im}(q_{j1}q_{k1}^* + q_{j2}q_{k2}^*)Z^\mu h_j\overleftrightarrow{\partial}_\mu h_k - \frac{1}{2}g\{iW_\mu^+[q_{k1}G^-\overleftrightarrow{\partial}^\mu h_k + q_{k2}e^{-i\theta_{23}}H^-\overleftrightarrow{\partial}^\mu h_k] + \mathrm{H.c.}\} \\ & + \left[ieA^\mu + \frac{ig}{c_W}\left(\frac{1}{2}-s_W^2\right)Z^\mu\right](G^+\overleftrightarrow{\partial}_\mu G^- + H^+\overleftrightarrow{\partial}_\mu H^-), \end{aligned} \tag{66}$$

where the repeated indices $j, k = 1, \ldots, 4$ are summed over. The neutral Goldstone boson interaction terms can be ascertained by taking $h_4 \equiv G^0$:

$$\mathcal{L}_{VG} = \left[\frac{1}{4}g^2 W_\mu^+ W^{\mu -} + \frac{g^2}{8c_W^2} Z_\mu Z^\mu\right] G^0 G^0 + \left\{\frac{1}{2} iegA^\mu W_\mu^+ G^- G^0 - \frac{ig^2 s_W^2}{2c_W} Z^\mu W_\mu^+ G^- G^0 + \text{H.c.}\right\} + \frac{g}{2c_W}\operatorname{Re}(q_{k1}) Z^\mu G^0 \overleftrightarrow{\partial}_\mu h_k + \frac{1}{2} g (W_\mu^+ G^- \overleftrightarrow{\partial}^\mu G^0 + W_\mu^- G^+ \overleftrightarrow{\partial}^\mu G^0). \quad (67)$$

Once again, we can verify by inspection that the Higgs boson-vector boson interactions are U(2)-invariant. Moreover, one can derive numerous relations among these couplings using the properties of the $q_{k\ell}$. In particular, Eqs. (36)–(38) imply the following relations among the Higgs boson-vector boson couplings [27–29]:

$$g(ZZh_j) = m_Z \sum_{k,\ell=1}^{3} \epsilon_{jk\ell}\, g(Zh_k h_\ell), \qquad (j = 1, 2, 3), \quad (68)$$

$$\sum_{k=1}^{3} [g(VVh_k)]^2 = \frac{g^2 m_V^4}{m_W^2}, \qquad V = W^\pm \quad \text{or} \quad Z, \quad (69)$$

$$\sum_{1\le j<k\le 3} [g(Zh_j h_k)]^2 = \frac{g^2}{4c_W^2}, \quad (70)$$

$$g(ZZh_j)g(ZZh_k) + 4m_Z^2 \sum_{\ell=1}^{3} g(Zh_j h_\ell) g(Zh_k h_\ell) = \frac{g^2 m_Z^2}{c_W^2}\delta_{jk}, \quad (71)$$

where the Feynman rules for the VVh_k and Zh_jh_kvertices are $ig^{\mu\nu} g(VVh_k)$ and $(p_k - p_j)^\mu g(Zh_jh_k)$, respectively, and the four-momenta p_j, p_k of the neutral Higgs bosons h_j, h_k point into the vertex.[11] Note that Eq. (71) holds for $j, k = 1, 2, 3, 4$.

VI. HIGGS COUPLINGS TO FERMIONS

The most general Yukawa couplings of Higgs bosons to fermions yield neutral Higgs-mediated flavor-changing neutral currents (FCNCs) at tree level [14,15]. Typically, these couplings are in conflict with the experimental bounds on FCNC processes. Thus, most model builders impose restrictions on the structure of the Higgs-fermion couplings to avoid the potential for phenomenological disaster. However, even in the case of the most general Higgs-fermion couplings, parameter regimes exist where FCNC effects are sufficiently under control. In the absence of new physics beyond the 2HDM, such parameter regimes are unnatural (but can be arranged with fine-tuning). In models such as the minimal supersymmetric extension of the standard model (MSSM), supersymmetry-breaking effects generate all possible Higgs-fermion Yukawa couplings allowed by electroweak gauge invariance. Nevertheless, the FCNC effects are one-loop suppressed and hence phenomenologically acceptable.

In this section, we will study the basis-independent description of the Higgs-fermion interaction. In a generic basis, the so-called type-III model [17,30] of Higgs-fermion interactions is governed by the following interaction Lagrangian:

$$-\mathcal{L}_Y = \bar{Q}_L^0 \tilde{\Phi}_1 \eta_1^{U,0} U_R^0 + \bar{Q}_L^0 \Phi_1 (\eta_1^{D,0})^\dagger D_R^0 + \bar{Q}_L^0 \tilde{\Phi}_2 \eta_2^{U,0} U_R^0 + \bar{Q}_L^0 \Phi_2 (\eta_2^{D,0})^\dagger D_R^0 + \text{H.c.}, \quad (72)$$

where $\Phi_{1,2}$ are the Higgs doublets, $\tilde{\Phi}_i \equiv i\sigma_2 \Phi_i^*$, Q_L^0 is the weak isospin quark doublet, and U_R^0, D_R^0 are weak isospin quark singlets. [The right and left-handed fermion fields are defined as: $\psi_{R,L} \equiv P_{R,L}\psi$, where $P_{R,L} \equiv \frac{1}{2}(1 \pm \gamma_5)$]. Here, Q_L^0, U_R^0, D_R^0 denote the interaction basis quark fields, which are vectors in the quark flavor space, and $\eta_1^{Q,0}$ and $\eta_2^{Q,0}$ $(Q = U, D)$ are four 3×3 matrices in quark flavor space. We have omitted the leptonic couplings in Eq. (72); these are obtained from Eq. (72) with the obvious substitutions $Q_L^0 \to L_L^0$ and $D_R^0 \to E_R^0$. (In the absence of right-handed neutrinos, there is no analog of U_R^0).

The derivation of the couplings of the physical Higgs bosons with the quark mass-eigenstates was given in Ref. [17] in the case of a *CP*-conserving Higgs sector. Here, we generalize that discussion to the more general case of a *CP*-violating Higgs sector. The first step is to identify the quark mass-eigenstates. This is accomplished by setting the scalar fields to their vacuum expectation values and performing unitary transformations of the left and right-handed up and down quark multiplets such that the resulting quark mass matrices are diagonal with non-negative entries. In more detail, we define left-handed and right-handed quark mass-eigenstate fields:

$$P_L U = V_L^U P_L U^0, \qquad P_R U = V_R^U P_R U^0, \qquad P_L D = V_L^D P_L D^0, \qquad P_R D = V_R^D P_R D^0, \quad (73)$$

and the Cabibbo-Kobayashi-Maskawa (CKM) matrix is defined by $K \equiv V_L^U V_L^{D\dagger}$. In addition, we introduce "rotated" Yukawa coupling matrices:

$$\eta_a^U \equiv V_L^U \eta_a^{U,0} V_R^{U\dagger}, \qquad \eta_a^D \equiv V_R^D \eta_a^{D,0} V_L^{D\dagger}, \quad (74)$$

(note the different ordering of V_L^Q and V_R^Q in the definitions

[11] The Feynman rule for the ZZh_k vertex includes a factor of 2 relative to the coefficient of the corresponding term in $i\mathcal{L}_{VVH}$ due to the identical Z bosons. The Feynman rule for the Zh_jh_k vertex is given by $\frac{1}{2}(g/c_W)\operatorname{Im}[q_{j1}q_{k1}^* + q_{j2}q_{k2}^*](p_k - p_j)^\mu$. Here, the factor of 2 relative to the corresponding term in Eq. (66) arises from the implicit double sum over j and k in the Lagrangian. Note that the rule for the Zh_jh_k vertex does not depend on the ordering of j and k.

of η_a^Q for $Q = U, D$). We then rewrite Eq. (72) in terms of the quark mass-eigenstate fields and the transformed couplings:

$$-\mathcal{L}_Y = \bar{Q}_L \tilde{\Phi}_{\bar{a}} \eta_a^U U_R + \bar{Q}_L \Phi_a \eta_{\bar{a}}^{D\dagger} D_R + \text{H.c.}, \qquad (75)$$

where $\eta_a^Q \equiv (\eta_1^Q, \eta_2^Q)$ is a vector with respect to the Higgs flavor-U(2) space. Under a U(2)-transformation of the scalar fields, $\eta_a^Q \to U_{a\bar{b}} \eta_b^Q$ and $\eta_{\bar{a}}^{Q\dagger} \to \eta_{\bar{b}}^{Q\dagger} U_{b\bar{a}}^\dagger$. Hence, the Higgs-quark Lagrangian is U(2)-invariant. We can construct basis-independent couplings following the strategy of section III by transforming to the Higgs basis. Using Eq. (11), we can rewrite Eq. (75) in terms of Higgs basis scalar fields:

$$\begin{aligned}-\mathcal{L}_Y = {} & \bar{Q}_L(\tilde{H}_1 \kappa^U + \tilde{H}_2 \rho^U) U_R \\ & + \bar{Q}_L (H_1 \kappa^{D\dagger} + H_2 \rho^{D\dagger}) D_R + \text{H.c.},\end{aligned} \qquad (76)$$

where

$$\kappa^Q \equiv \hat{v}_{\bar{a}}^* \eta_a^Q, \qquad \rho^Q \equiv \hat{w}_{\bar{a}}^* \eta_a^Q. \qquad (77)$$

Inverting Eq. (77) yields:

$$\eta_a^Q = \kappa^Q \hat{v}_a + \rho^Q \hat{w}_a. \qquad (78)$$

Under a U(2) transformation, κ^Q is invariant, whereas ρ^Q is a pseudoinvariant that transforms as

$$\rho^Q \to (\det U) \rho^Q. \qquad (79)$$

By construction, κ^U and κ^D are proportional to the (real non-negative) diagonal quark mass matrices M_U and M_D, respectively. In particular, the M_Q are obtained by inserting Eq. (12) into Eq. (76), which yields:

$$M_U = \frac{v}{\sqrt{2}} \kappa^U = \text{diag}(m_u, m_c, m_t) = V_L^U M_U^0 V_R^{U\dagger}, \qquad (80)$$

$$M_D = \frac{v}{\sqrt{2}} \kappa^{D\dagger} = \text{diag}(m_d, m_s, m_b) = V_L^D M_D^0 V_R^{D\dagger}, \qquad (81)$$

where $M_U^0 \equiv (v/\sqrt{2}) \hat{v}_{\bar{a}}^* \eta_a^{U,0}$ and $M_D^0 \equiv (v/\sqrt{2}) \hat{v}_a \eta_{\bar{a}}^{D,0\dagger}$. That is, we have chosen the unitary matrices V_L^U, V_R^U, V_L^D, and V_R^D such that M_D and M_U are diagonal matrices with real non-negative entries.[12] In contrast, the ρ^Q are independent complex 3×3 matrices.

In order to obtain the interactions of the physical Higgs bosons with the quark mass-eigenstates, we do not require the intermediate step involving the Higgs basis. Instead, we insert Eq. (46) into Eq. (75) and obtain:

[12] This can be accomplished by the singular-value decompositions of the complex matrices M_U^0 and M_D^0 [31].

$$\begin{aligned}-\mathcal{L}_Y = {} & \frac{1}{v} \bar{D} \Big\{ M_D (q_{k1} P_R + q_{k1}^* P_L) \\ & + \frac{v}{\sqrt{2}} [q_{k2} [e^{i\theta_{23}} \rho^D]^\dagger P_R + q_{k2}^* e^{i\theta_{23}} \rho^D P_L] \Big\} D h_k \\ & + \frac{1}{v} \bar{U} \Big\{ M_U (q_{k1} P_L + q_{k1}^* P_R) \\ & + \frac{v}{\sqrt{2}} [q_{k2}^* e^{i\theta_{23}} \rho^U P_R + q_{k2} [e^{i\theta_{23}} \rho^U]^\dagger P_L] \Big\} U h_k \\ & + \Big\{ \bar{U} [K [\rho^D]^\dagger P_R - [\rho^U]^\dagger K P_L] D H^+ \\ & + \frac{\sqrt{2}}{v} \bar{U} [K M_D P_R - M_U K P_L] D G^+ + \text{H.c.} \Big\},\end{aligned} \qquad (82)$$

where $k = 1, \ldots 4$. Since $e^{i\theta_{23}} \rho^Q$ and $[\rho^Q]^\dagger H^+$ are $U(2)$-invariant, it follows that Eq. (82) is a basis-independent representation of the Higgs-quark interactions.

The neutral Goldstone boson interactions ($h_4 \equiv G^0$) are easily isolated:

$$-\mathcal{L}_{YG} = \frac{i}{v} [\bar{D} M_D \gamma_5 D - \bar{U} M_U \gamma_5 U] G^0. \qquad (83)$$

In addition, since the q_{k1} are real for $k = 1, 2, 3$, it follows that the piece of the neutral Higgs-quark couplings proportional to the quark mass matrix is of the form $v^{-1} \bar{Q} M_Q q_{k1} Q h_k$.

The couplings of the neutral Higgs bosons to quark pairs are generically CP-violating as a result of the complexity of the q_{k2} and the fact that the matrices $e^{i\theta_{23}} \rho^Q$ are not generally hermitian or anti-Hermitian. (Invariant conditions for the CP-invariance of these couplings are given in Appendix D). Equation (82) also exhibits Higgs-mediated FCNCs at tree level by virtue of the fact that the ρ^Q are not flavor-diagonal. Thus, for a phenomenologically acceptable theory, the off-diagonal elements of ρ^Q must be small.

VII. THE SIGNIFICANCE OF $\tan\beta$

In Secs. V and VI, we have written out the entire interaction Lagrangian for the Higgs bosons of the 2HDM. Yet, the famous parameter $\tan\beta$, given by $\tan\beta \equiv v_2/v_1$ in a generic basis [see Eq. (3)], does not appear in any physical Higgs (or Goldstone) boson coupling. This is rather surprising given the large literature of 2HDM phenomenology in which the parameter $\tan\beta$ is ubiquitous. For example, numerous methods have been proposed for measuring $\tan\beta$ at future colliders [32–39]. In a generic basis, one can also define the relative phase of the two vacuum expectation values, $\xi = \arg(v_2 v_1^*)$. However, neither $\tan\beta$ nor ξ are basis-independent. One can remove ξ by rephasing one of the two-Higgs-doublet fields, and both ξ and $\tan\beta$ can be removed entirely by transforming to the Higgs basis. Thus, in a general 2HDM, $\tan\beta$ is an unphysical parameter with no significance *a priori*.

The true significance of $\tan\beta$ emerges only in specialized versions of the 2HDM, where $\tan\beta$ is promoted to a physical parameter. As noted in Sec. VI, the general 2HDM generally predicts FCNCs in conflict with experimental data. One way to avoid this phenomenological problem is to constrain the theoretical structure of the 2HDM. Such constraints often pick out a preferred basis. Relative to that basis, $\tan\beta$ is then a meaningful parameter.

The most common 2HDM constraint is the requirement that some of the Higgs-fermion Yukawa couplings vanish in a "preferred" basis. This leads to the well-known type-I and type-II 2HDMs [12] (henceforth called 2HDM-I and 2HDM-II). In the 2HDM-I, there exists a preferred basis where $\eta_2^U = \eta_2^D = 0$ [10,12]. In the 2HDM-II, there exists a preferred basis where $\eta_1^U = \eta_2^D = 0$ [11,12]. These conditions can be enforced by a suitable symmetry. For example, the MSSM possesses a type-II Higgs-fermion interaction, in which case the supersymmetry guarantees that $\eta_1^U = \eta_2^D = 0$. In nonsupersymmetric models, appropriate discrete symmetries can be found to enforce the type-I or type-II Higgs-fermion couplings.[13]

The conditions for type-I and type-II Higgs-fermion interactions given above are basis-dependent. But, there is also a basis-independent criterion that was first given in Ref. [17][14]:

$$\epsilon_{\bar{a}\bar{b}}\eta_a^D\eta_b^U = \epsilon_{ab}\eta_{\bar{a}}^{D\dagger}\eta_{\bar{b}}^{U\dagger} = 0, \qquad \text{type-I,} \tag{84}$$

$$\delta_{a\bar{b}}\eta_{\bar{a}}^{D\dagger}\eta_b^U = 0, \qquad \text{type-II.} \tag{85}$$

We can now prove that $\tan\beta$ is a physical parameter in the 2HDM-II (we leave the corresponding analysis for the 2HDM-I to the reader[15]). In the preferred basis where $\eta_1^U = \eta_2^D = 0$, we shall denote: $\hat{v} = e^{i\eta}(\cos\beta, \sin\beta e^{i\xi})$ and $\hat{w} = e^{-i\eta}(-\sin\beta e^{-i\xi}, \cos\beta)$. Evaluating $\kappa^Q = \hat{v}^* \cdot \eta^Q$ and $\rho^Q = \hat{w}^* \cdot \eta^Q$ in the preferred basis, and recalling that the κ^Q are diagonal real matrices, it follows that

$$\boldsymbol{I}\, e^{-i(\xi+2\eta)}\tan\beta = -\rho^{D\dagger}(\kappa^D)^{-1} = (\rho^U)^{-1}\kappa^U, \tag{86}$$

where $\boldsymbol{I}$ is the identity matrix in quark flavor space and $\kappa^Q = \sqrt{2}M_Q/v$ [see Eqs. (80) and (81)]. These two definitions are consistent if $\kappa^D\kappa^U + \rho^{D\dagger}\rho^U = 0$ is satisfied. But the latter is equivalent to the type-II condition [which can be verified by inserting Eq. (78) into Eq. (85)].

To understand the phase factor that appears in Eq. (86), we note that only unitary matrices of the form $U = \mathrm{diag}(e^{i\chi_1}, e^{i\chi_2})$ that span a $\mathrm{U}(1)\times\mathrm{U}(1)$ subgroup of the flavor-U(2) group preserve the type-II conditions $\eta_1^U = \eta_2^D = 0$ in the preferred basis. Under transformations of this type, $\eta \to \eta + \chi_1$ and $\xi \to \xi + \chi_2 - \chi_1$. Using Eq. (79), it follows that $\rho^Q \to e^{i(\chi_1+\chi_2)}\rho^Q$. Hence $\rho^Q e^{-i(\xi+2\eta)}$ is invariant with respect to such $\mathrm{U}(1)\times\mathrm{U}(1)$ transformations. We conclude that Eq. (86) is covariant with respect to transformations that preserve the type-II condition.

The conditions specified in Eq. (86) are quite restrictive. In particular, they determine the matrices ρ^Q:

$$\rho^D e^{-i(\xi+2\eta)} = \frac{-\sqrt{2}M_D\tan\beta}{v}, \qquad \rho^U e^{-i(\xi+2\eta)} = \frac{\sqrt{2}M_U\cot\beta}{v}. \tag{87}$$

Up to an overall phase, ρ^U and ρ^D are real diagonal matrices with non-negative entries. There is also some interesting information in the phase factors of Eq. (87). Although the ρ^Q are pseudoinvariants, we have noted below Eq. (82) that $e^{i\theta_{23}}\rho^Q$ is U(2)-invariant. This means that the phase factor $e^{-i(\theta_{23}+\xi+2\eta)}$ is a physical parameter. Moreover, we can now define $\tan\beta$ as a physical parameter of the 2HDM-II as follows:

$$\tan\beta = \frac{v}{3\sqrt{2}}|\mathrm{Tr}(\rho^D M_D^{-1})|, \tag{88}$$

where $0 \le \beta \le \pi/2$. This is a manifestly basis-independent definition, so $\tan\beta$ is indeed physical.

In Higgs studies at future colliders, suppose one encounters phenomena that appear consistent with a 2HDM. It may not be readily apparent that there is any particular structure in the Higgs-fermion interactions. In particular, it could be that Eq. (86) is simply false. A safe strategy is to always measure physical quantities, which must be U(2)-invariant. Here is a modest proposal, assuming that the Yukawa couplings of the Higgs bosons to the third-generation fermions dominate, in which case we can ignore the effects of the first two generations.[16] In a one-generation model, one can introduce three $\tan\beta$-like parameters

$$\tan\beta_b \equiv \frac{v}{\sqrt{2}}\frac{|\rho^D|}{m_b}, \qquad \tan\beta_t \equiv \frac{\sqrt{2}}{v}\frac{m_t}{|\rho^U|}, \qquad \tan\beta_\tau \equiv \frac{v}{\sqrt{2}}\frac{|\rho^E|}{m_\tau}, \tag{89}$$

[13]These discrete symmetries also imply that some of the coefficients of the scalar potential must also vanish in the same preferred basis [10–13].

[14]In this paper, we have slightly modified our definition of the Yukawa coupling. What is called η^D in Ref. [17] is called $\eta^{D\dagger}$ here.

[15]Equation (84) involves pseudoinvariant quantities. Nevertheless, setting these quantities to zero yields a U(2)-invariant condition.

[16]This is probably not a bad assumption, since κ^Q is proportional to the quark mass matrix M_Q.

where $\tan\beta_\tau$ is analogous to $\tan\beta_d$ and depends on the third-generation Higgs-lepton interaction. In a type-II model, one indeed has $\tan\beta_b = \tan\beta_t = \tan\beta_\tau = \tan\beta$. In the more general (type-III) 2HDM, there is no reason for the three parameters above to coincide. However, these three parameters are indeed U(2)-invariant quantities, and thus correspond to physical observables that can be measured in the laboratory. The interpretation of these parameters is straightforward. In the Higgs basis, up and down-type quarks interact with both Higgs doublets. But, clearly there exists some basis (i.e., a rotation by an angle β_t from the Higgs basis) for which only one of the two up-type quark Yukawa couplings is nonvanishing. This defines the physical angle β_t. The interpretation of the other two angles is similar.

Since the phase of $e^{i\theta_{23}}\rho^Q$ is a physical parameter, one can generalize Eq. (89) by defining

$$e^{i(\theta_{23}-\chi_b)}\tan\beta_b \equiv \frac{v}{\sqrt{2}}\frac{\rho^{D*}}{m_b},\qquad e^{i(\theta_{23}-\chi_t)}\tan\beta_t \equiv \frac{\sqrt{2}}{v}\frac{m_t}{\rho^U},\tag{90}$$

and similarly for $\tan\beta_\tau$. Thus, in addition to three $\tan\beta$-like parameters, there are three independent physical phases χ_b, χ_t, and χ_τ that could in principle be deduced from experiment. Of course, in the 2HDM-II, one must have $\beta_b = \beta_t = \beta_\tau$ and $\chi_b = \chi_t = \chi_\tau$.

A similar analysis can be presented for the case of the 2HDM-I. In this case, one is led to define slightly different $\tan\beta$-like physical parameters. But, these would be related to those defined in Eq. (89) in a simple way. A particular choice could be motivated if one has evidence that that either the type-I or type-II conditions are approximately satisfied.

We conclude this section by illustrating the utility of this approach in the case of the MSSM. This example has already been presented in Ref. [17] in the case of a CP-conserving Higgs sector. We briefly explain how that analysis is generalized in the case of a CP-violating Higgs sector. The MSSM Higgs sector is a CP-conserving type-II 2HDM in the limit of exact supersymmetry. However, when supersymmetry-breaking effects are taken into account, loop corrections to the Higgs potential and the Higgs-fermion interactions can lead to both CP-violating effects in the Higgs sector, and the (radiative) generation of the Higgs-fermion Yukawa couplings that are absent in the type-II limit. In particular, in the approximation that supersymmetric masses are significantly larger than m_Z, the effective Lagrangian that describes the coupling of the Higgs bosons to the third-generation quarks is given (in the notation of [6]) by

$$-\mathcal{L}_{\rm eff} = (h_b+\delta h_b)(\bar{q}_L\Phi_1)b_R + (h_t+\delta h_t)(\bar{q}_L\tilde{\Phi}_2)t_R + \Delta h_b(\bar{q}_L\Phi_2)b_R + \Delta h_t(\bar{q}_L\tilde{\Phi}_1)t_R + \text{H.c.},\tag{91}$$

where $\bar{q}_L \equiv (\bar{u}_L, \bar{d}_L)$. Note that the terms proportional to Δh_b and Δh_t, which are absent in the tree-level MSSM, are generated at one-loop due to supersymmetry-breaking effects Thus, we identify $\eta^D = ((h_b+\delta h_b)^*, \Delta h_b^*)$ and $\eta^U = (\Delta h_t, h_t+\delta h_t)$. The tree-level MSSM is CP-conserving, and $\xi = 0$ in the supersymmetric basis. At one-loop, CP-violating effects can shift ξ away from zero, and we shall denote this quantity by $\Delta\xi$.[17] Evaluating $\kappa^Q = \hat{v}^*\cdot\eta^Q$ and $\rho^Q = \hat{w}^*\cdot\eta^Q$ as we did above Eq. (86),

$$\begin{aligned} e^{i\eta}\kappa^D &= c_\beta(h_b+\delta h_b)^* + e^{-i\Delta\xi}s_\beta(\Delta h_b)^*,\\ e^{-i\eta}\rho^D &= -e^{i\Delta\xi}s_\beta(h_b+\delta h_b)^* + c_\beta(\Delta h_b)^*,\end{aligned}\tag{92}$$

$$\begin{aligned} e^{i\eta}\kappa^U &= c_\beta\Delta h_t + e^{-i\Delta\xi}s_\beta(h_t+\delta h_t),\\ e^{-i\eta}\rho^U &= -e^{i\Delta\xi}s_\beta\Delta h_t + c_\beta(h_t+\delta h_t).\end{aligned}\tag{93}$$

By definition, the κ^Q are real and non-negative, and related to the top and bottom quark masses via Eqs. (80) and (81). Thus, the tree-level relations between m_b, m_t and h_b, h_t respectively are modified [40][18]:

$$\begin{aligned} m_b &= \frac{v\kappa^D}{\sqrt{2}} = \frac{vc_\beta h_b}{\sqrt{2}}\left[1+\text{Re}\left(\frac{\delta h_b}{h_b}+\frac{\Delta h_b}{h_b}e^{i\Delta\xi}\tan\beta\right)\right]\\ &\equiv \frac{vc_\beta h_b}{\sqrt{2}}[1+\text{Re}(\Delta_b)],\end{aligned}\tag{94}$$

$$\begin{aligned} m_t &= \frac{v\kappa^U}{\sqrt{2}} = \frac{vs_\beta h_t}{\sqrt{2}}\left[1+\text{Re}\left(\frac{\delta h_t}{h_t}+\frac{\Delta h_t}{h_t}e^{i\Delta\xi}\cot\beta\right)\right]\\ &\equiv \frac{vs_\beta h_t}{\sqrt{2}}[1+\text{Re}(\Delta_t)],\end{aligned}\tag{95}$$

which define the complex quantities Δ_b and Δ_t.[19]

Equation (90) then yields:

$$\begin{aligned} \tan\beta_b &= \left|\frac{-e^{-i\Delta\xi}s_\beta(h_b+\delta h_b)+c_\beta\Delta h_b}{c_\beta(h_b+\delta h_b)+e^{i\Delta\xi}s_\beta\Delta h_b}\right|,\\ \chi_b &= \theta_{23}+\psi_b+\eta,\end{aligned}\tag{96}$$

[17] In practice, one would rephase the fields after computing the radiative corrections. But, since we are advocating basis-independent methods in this paper, there is no need for us to do this.

[18] If one of the Higgs fields is rephased in order to remove the phase $\Delta\xi$, then one simultaneously rephases $\Delta h_{b,t}$ such that the quantities $\Delta h_{b,t}e^{i\Delta\xi}$ are invariant with respect to the rephasing. In particular, h_b and h_t are not rephased, since these tree-level quantities are always real and positive and proportional to the tree-level values of m_b and m_t, respectively.

[19] In deriving Eqs. (94) and (95), we computed $\kappa^Q = |\kappa^Q|$ by expanding up to linear order in the one-loop quantities $\Delta h_{b,t}$ and $\delta h_{b,t}$. Explicit expressions for Δ_b and Δ_t in terms of supersymmetric masses and parameters, and references to the original literature can be found in Ref. [6].

$$\tan\beta_t = \left|\frac{c_\beta \Delta h_t + e^{-i\Delta\xi} s_\beta (h_t + \delta h_t)}{-\Delta h_t s_\beta e^{i\Delta\xi} + c_\beta (h_t + \delta h_t)}\right|,$$
$$\chi_t = \theta_{23} + \psi_t + \eta, \tag{97}$$

where $\psi_{t,b} \equiv \arg(e^{-i\eta}\rho^{U,D})$. Expanding the numerators and denominators above and dropping terms of quadratic order in the one-loop quantities, we end up with

$$\tan\beta_b = \frac{\tan\beta}{1 + \mathrm{Re}\Delta_b}\left[1 + \frac{1}{s_\beta^2}\mathrm{Re}\left(\frac{\delta h_b}{h_b} - c_\beta^2 \Delta_b\right)\right], \tag{98}$$

$$\cot\beta_t = \frac{\cot\beta}{1 + \mathrm{Re}\Delta_t}\left[1 + \mathrm{Re}\left(\Delta_t - \frac{1}{c_\beta s_\beta}\frac{\Delta h_t}{h_t} e^{i\Delta\xi}\right)\right]. \tag{99}$$

We have chosen to write $\tan\beta_b/\tan\beta$ in terms of Δ_b and $\delta h_b/h_b$, and $\cot\beta_t/\cot\beta$ in terms of Δ_t and $\Delta h_t/h_t$ in order to emphasize the large $\tan\beta$ behavior of the deviations of these quantities from one. In particular, keeping only the leading $\tan\beta$-enhanced corrections, Eqs. (94) and (95) imply that[20]

$$\Delta_b \simeq e^{i\Delta\xi}\frac{\Delta h_b}{h_b}\tan\beta, \qquad \Delta_t \simeq \frac{\delta h_t}{h_t}. \tag{100}$$

That is, the complex quantity Δ_b is $\tan\beta$-enhanced. In typical models at large $\tan\beta$, the quantity $|\Delta_b|$ can be of order 0.1 or larger and of either sign. Thus, keeping only the one-loop corrections that are $\tan\beta$-enhanced,[21]

$$\tan\beta_b \simeq \frac{\tan\beta}{1 + \mathrm{Re}\Delta_b},$$
$$\cot\beta_t \simeq \cot\beta\left[1 - \tan\beta\,\mathrm{Re}\left(\frac{\Delta h_t}{h_t} e^{i\Delta\xi}\right)\right]. \tag{101}$$

Thus, we have expressed the basis-independent quantities $\tan\beta_b$ and $\tan\beta_t$ in terms of parameters that appear in the natural basis of the MSSM Higgs sector. Indeed, we find that $\tan\beta_b \neq \tan\beta_t$ as a consequence of supersymmetry-breaking loop-effects.

VIII. DISCUSSION AND CONCLUSIONS

In this paper, we have completed the theoretical development of the basis-independent treatment of the two-Higgs-doublet model (2HDM) that was initiated in Ref. [17]. In particular, we focused on the construction of quantities that are invariant with respect to global U(2) transformations of the form $\Phi_a \to U_{a\bar{b}}\Phi_b$. Such invariant quantities are basis-independent and can therefore be associated with the physical parameters of the model. We have also emphasized the utility of pseudoinvariant quantities that are modified by a phase factor (equal to some integer power of det$U$) under U(2)-transformations. Although such quantities are not observables, any two of them can be combined to form an invariant quantity.

The main accomplishment of this paper was the treatment of the Higgs mass-eigenstates that allows for the most general set of CP-violating Higgs couplings. In this most general case, three neutral Higgs states mix to yield three neutral Higgs mass-eigenstates of indefinite CP. The neutral Higgs sector is parameterized by three physical masses and three mixing angles. The masses are, of course, U(2)-invariant quantities. We have demonstrated how to define the three mixing angles such that two of the three angles are invariant and one is a pseudoinvariant quantity. We then identified the invariants that directly enter the various Higgs couplings to bosons and fermions of the model. The end result is a complete listing of all Higgs interactions in an invariant basis-independent form.

Using the above results, we addressed the significance of the parameter $\tan\beta$, which appears in many of the Higgs boson Feynman rules in the generic-basis formulation of the 2HDM [5]. Since $\tan\beta$ is a basis-dependent quantity, the appearance of $\tan\beta$ in the Higgs Feynman boson rules is an illusion. In fact, $\tan\beta$ is completely absent in the invariant basis-independent form of the Feynman rules. For example, we demonstrated that in the one-generation model, the Higgs-fermion Feynman rules depend on three separate $\tan\beta$-like parameters. However, in contrast to $\tan\beta$, these three separate parameters are U(2)-invariant quantities that depend on physical Higgs-fermion couplings. If one imposes constraints on the Higgs Lagrangian such as a discrete symmetry $\Phi_1 \to \Phi_1$ and $\Phi_2 \to -\Phi_2$ (in some basis), or supersymmetry (which selects a preferred basis), then $\tan\beta$ is promoted to a physical parameter. The latter can then be explicitly associated with an invariant quantity of the basis-independent formalism.

With the basis-independent formalism now fully developed, it is now time to begin to apply these ideas to the precision Higgs programs at future colliders. Instead of studying how to make precision measurements of $\tan\beta$ (which does not make sense in the general 2HDM context), one should examine the potential for precision measurements of physical [U(2)-invariant] parameters. In precision studies of the Higgs-fermion interactions, it ought to be possible to make measurements of the three $\tan\beta$-like parameters introduced in Sec. VII. Close to the decoupling limit [42,43], the lightest neutral Higgs boson h_1 of the 2HDM is nearly indistinguishable from the standard model CP-even Higgs boson. Consequently, the couplings of h_1 are expected to be quite insensitive to $\tan\beta$. To extract experimental information on the $\tan\beta$-like parameters will therefore require the observation of the heavier Higgs bosons h_2, h_3, and $H^\pm$.

For example, if h_2, h_3 are kinematically accessible at the ILC, then one can probe the values of $\tan\beta_f$ [$f = t$, b, and

[20]Because the one-loop corrections δh_b, Δh_b, δh_t, and Δh_t depend only on Yukawa and gauge couplings and the supersymmetric particle masses, they contain no hidden $\tan\beta$ enhancements or suppressions [41].

[21]In Ref. [17] the one-loop $\tan\beta$-enhanced correction to $\cot\beta_t$ was incorrectly omitted.

τ] by studying Higgs production (in both e^+e^- and $\gamma\gamma$ collisions) and Higgs decay processes that involve b-quarks, t-quarks, and τ-leptons. Studies of $b\bar{b}h_k$ [34,35], $t\bar{t}h_k$ [34], and $\tau^+\tau^-$ [38] production provide initial estimates for the sensitivity to $\tan\beta$. The production of $t\bar{b}H^-$ [32,37], exhibits dependence on both $\tan\beta_t$ and $\tan\beta_b$, although the latter dependence dominates if $\tan\beta_b \gg 1$. The $\tan\beta$-like parameters can also be probed by precision studies of the heavy Higgs boson decays to heavy fermion pairs. In particular, observation of $H^\pm \to \tau^\pm\nu_\tau$ would provide independent information on the value of $\tan\beta_\tau$. Opportunities also exist to study the couplings of the heavy Higgs bosons to fermion pairs at the LHC if $\tan\beta$ is large [6]. In Ref. [39], $gg \to b\bar{b}h_{2,3}$ followed by $h_{2,3} \to \tau^+\tau^-$ provides an excellent channel for measuring $\tan\beta$. A number of $\tan\beta$-enhanced effects that govern various b-quark decay processes can also provide useful information on $\tan\beta_b$ and $\tan\beta_\ell$ ($\ell = \tau$ or μ). Perhaps the most sensitive process of this kind is the rare (one-loop induced) decay $B_s \to \mu^+\mu^-$, whose rate is enhanced in the MSSM by a factor of $\tan^6\beta$ [44].

It remains to be seen how effective the processes outlined above are for distinguishing among the various $\tan\beta$-like parameters. If the three $\tan\beta$-like parameters are found to be close in value, this result would provide an important clue to possible constraints underlying the theoretical structure of the 2HDM. In particular, small deviations among these parameters could be related to new TeV-scale physics associated with the Higgs sector. A particular example of this in the context of the MSSM was given at the end of Sec. VII. The application of the methods of this paper to the study of precision measurements of the $\tan\beta$-like parameters at future colliders will be treated in more detail elsewhere.

The potential phenomenological implications of the flavor structure of the full three-generation model has not yet been examined in a comprehensive way. Strictly speaking, in the three-generation model, the three $\tan\beta$-like parameters mentioned above would have to be replaced with a more complicated set of parameters that reflect the full flavor structure of the Higgs-fermion interactions. Since the third-generation Higgs-fermion interactions are expected to dominate, the one-generation results should provide a reasonable first approximation. However, the absence of large FCNC phenomena imposes some significant restrictions on the Higgs-fermion interactions of the most general 2HDM. A basis-independent analysis of these restrictions will be addressed in a separate publication.

In conclusion, the basis-independent formalism provides a powerful approach for connecting physical observables that can be measured in the laboratory with fundamental invariant parameters of the 2HDM. This will permit the development of two-Higgs-doublet model-independent analyses of data in Higgs studies at the LHC, ILC and beyond. Ultimately, if 2HDM phenomena are discovered at future colliders, such analyses will provide the most general setting for identifying the fundamental nature of the 2HDM dynamics.

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APPENDIX A: THE 2HDM SCALAR POTENTIAL IN A GENERIC BASIS

Let Φ_1 and Φ_2 denote two complex hypercharge-one, $SU(2)_L$ doublets of scalar fields. The most general gauge-invariant scalar potential is given by

$$\begin{aligned}\mathcal{V} = {}& m_{11}^2\Phi_1^\dagger\Phi_1 + m_{22}^2\Phi_2^\dagger\Phi_2 - [m_{12}^2\Phi_1^\dagger\Phi_2 + \text{H.c.}] \\ &+ \tfrac{1}{2}\lambda_1(\Phi_1^\dagger\Phi_1)^2 + \tfrac{1}{2}\lambda_2(\Phi_2^\dagger\Phi_2)^2 + \lambda_3(\Phi_1^\dagger\Phi_1)(\Phi_2^\dagger\Phi_2) \\ &+ \lambda_4(\Phi_1^\dagger\Phi_2)(\Phi_2^\dagger\Phi_1) + \{\tfrac{1}{2}\lambda_5(\Phi_1^\dagger\Phi_2)^2 \\ &+ [\lambda_6(\Phi_1^\dagger\Phi_1) + \lambda_7(\Phi_2^\dagger\Phi_2)]\Phi_1^\dagger\Phi_2 + \text{H.c.}\},\end{aligned} \tag{A1}$$

where m_{11}^2, m_{22}^2, and $\lambda_1, \cdots, \lambda_4$ are real parameters. In general, m_{12}^2, λ_5, λ_6, and λ_7 are complex. The form of Eq. (A1) holds for any generic choice of $\Phi_1 - \Phi_2$ basis, whereas the coefficients m_{ij}^2 and λ_i are basis-dependent quantities. Matching Eq. (A1) to the U(2)-covariant form of Eq. (2), we identify:

$$\begin{aligned} Y_{11} &= m_{11}^2, \qquad Y_{12} = -m_{12}^2, \\ Y_{21} &= -(m_{12}^2)^*, \qquad Y_{22} = m_{22}^2,\end{aligned} \tag{A2}$$

and

$$\begin{aligned} Z_{1111} &= \lambda_1, & Z_{2222} &= \lambda_2, \\ Z_{1122} &= Z_{2211} = \lambda_3, & Z_{1221} &= Z_{2112} = \lambda_4, \\ Z_{1212} &= \lambda_5, & Z_{2121} &= \lambda_5^*, \\ Z_{1112} &= Z_{1211} = \lambda_6, & Z_{1121} &= Z_{2111} = \lambda_6^*, \\ Z_{2212} &= Z_{1222} = \lambda_7, & Z_{2221} &= Z_{2122} = \lambda_7^*. \end{aligned} \tag{A3}$$

Explicit formulae for the coefficients of the Higgs basis scalar potential in terms of the corresponding coefficients of Eq. (A1) in a generic basis can be found in Ref. [17].

APPENDIX B: THE NEUTRAL HIGGS BOSON SQUARED-MASS MATRIX IN A GENERIC BASIS

Starting from Eq. (2), one can obtain the neutral Higgs squared-mass matrix from the quadratic part of the scalar potential:

$$\mathcal{V}_{\rm mass} = \frac{1}{2}(\Phi_a^0 \quad \Phi_{\bar{b}}^{0\dagger})\boldsymbol{M}^2\begin{pmatrix}\Phi_{\bar{c}}^{0\dagger}\\ \Phi_d^0\end{pmatrix}. \tag{B1}$$

Thus, $\boldsymbol{M}^2$ is given by the following matrix of second derivatives:

$$\boldsymbol{M}^2 = \begin{pmatrix} \frac{\partial^2\mathcal{V}}{\partial\Phi_a^0\partial\Phi_{\bar{c}}^{0\dagger}} & \frac{\partial^2\mathcal{V}}{\partial\Phi_a^0\partial\Phi_d^0}\\ \frac{\partial^2\mathcal{V}}{\partial\Phi_{\bar{b}}^{0\dagger}\partial\Phi_{\bar{c}}^{0\dagger}} & \frac{\partial^2\mathcal{V}}{\partial\Phi_{\bar{b}}^{0\dagger}\partial\Phi_d^0}\end{pmatrix}_{\Phi_a^0=v_a}, \tag{B2}$$

where $v_a \equiv v\hat{v}_a/\sqrt{2}$ and $\hat{v}_{\bar{a}}^*\hat{v}_a = 1$. With $\mathcal{V}$ given by Eq. (2), one finds:

$$\boldsymbol{M}^2 = \begin{pmatrix} (Y_{a\bar{c}})^* + \frac{1}{2}v^2[(Z_{a\bar{c}f\bar{e}} + Z_{f\bar{c}a\bar{e}})\hat{v}_e\hat{v}_{\bar{f}}^*]^* & \frac{1}{4}v^2(Z_{e\bar{a}f\bar{d}} + Z_{e\bar{d}f\bar{a}})\hat{v}_{\bar{e}}^*\hat{v}_{\bar{f}}^*\\ \frac{1}{4}v^2(Z_{b\bar{e}c\bar{f}} + Z_{c\bar{e}b\bar{f}})\hat{v}_e\hat{v}_f & Y_{b\bar{d}} + \frac{1}{2}v^2(Z_{e\bar{f}b\bar{d}} + Z_{e\bar{d}b\bar{f}})\hat{v}_{\bar{e}}^*\hat{v}_f\end{pmatrix}. \tag{B3}$$

In deriving this result, we used the hermiticity properties of Y and Z to rewrite the upper left hand block so that the indices appear in the standard order for matrix multiplication in Eq. (B1). In addition, we employed:

$$\frac{\partial\Phi_e^0}{\partial\Phi_a^0} = \delta_{e\bar{a}}, \qquad \frac{\partial\Phi_{\bar{f}}^{0\dagger}}{\partial\Phi_{\bar{b}}^{0\dagger}} = \delta_{b\bar{f}}. \tag{B4}$$

It is convenient to express the squared-mass matrix in terms of (pseudo)-invariants. To do this, we note that we can expand an Hermitian second-ranked tensor [which satisfies $A_{a\bar{b}} = (A_{b\bar{a}})^*$] in terms of the eigenvectors of $V_{a\bar{b}} \equiv \hat{v}_a\hat{v}_{\bar{b}}^*$:

$$A_{a\bar{b}} = \mathrm{Tr}(VA)V_{a\bar{b}} + \mathrm{Tr}(WA)W_{a\bar{b}} + [(\hat{v}_{\bar{c}}^*\hat{w}_dA_{c\bar{d}})\hat{v}_a\hat{w}_{\bar{b}}^* + (\hat{w}_{\bar{c}}^*\hat{v}_dA_{c\bar{d}})\hat{w}_a\hat{v}_{\bar{b}}^*], \tag{B5}$$

where $W_{a\bar{b}} \equiv \hat{w}_a\hat{w}_{\bar{b}}^* = \delta_{a\bar{b}} - V_{a\bar{b}}$. Likewise, we can expand a second-ranked symmetric tensor with two unbarred (or two barred indices), e.g.,

$$A_{ab} = (\hat{v}_{\bar{c}}^*\hat{v}_{\bar{d}}^*A_{cd})\hat{v}_a\hat{v}_b + (\hat{w}_{\bar{c}}^*\hat{w}_{\bar{d}}^*A_{cd})\hat{w}_a\hat{w}_b + (\hat{v}_{\bar{c}}^*\hat{w}_{\bar{d}}^*A_{cd})(\hat{v}_a\hat{w}_b + \hat{w}_a\hat{v}_b). \tag{B6}$$

We can therefore rewrite the upper and lower right-hand 2×2 blocks of the squared-mass matrix [Eq. (B3)], respectively, as

$$[\boldsymbol{M}^2]_{\bar{a}\bar{d}} = \tfrac{1}{2}v^2[Z_1\hat{v}_{\bar{a}}^*\hat{v}_{\bar{d}}^* + Z_5\hat{w}_{\bar{a}}^*\hat{w}_{\bar{d}}^* + Z_6(\hat{v}_{\bar{a}}^*\hat{w}_{\bar{d}}^* + \hat{w}_{\bar{a}}^*\hat{v}_{\bar{d}}^*)], \tag{B7}$$

$$[\boldsymbol{M}^2]_{b\bar{d}} = (Y_1 + Z_1v^2)V_{b\bar{d}} + [Y_2 + \tfrac{1}{2}(Z_3 + Z_4)v^2]W_{b\bar{d}} + [(Y_3 + Z_6v^2)\hat{v}_b\hat{w}_{\bar{d}}^* + (Y_3^* + Z_6^*v^2)\hat{w}_b\hat{v}_{\bar{d}}^*]. \tag{B8}$$

The upper and lower left hand blocks are then given by the Hermitian adjoints of the lower and upper right-hand blocks, respectively. Note that Eq. (B8) can be simplified further by eliminating Y_1 and Y_3 using the scalar potential minimum conditions [Eq. (21)].

Let us apply this result to the Higgs bases, where $\hat{v} = (1, 0)$ and $\hat{w} = (0, 1)$. After imposing the scalar potential minimum conditions,

$$\boldsymbol{M}^2 = \frac{1}{2}v^2\begin{pmatrix} Z_1 & Z_6^* & Z_1 & Z_6\\ Z_6 & Z_3+Z_4+2Y_2/v^2 & Z_6 & Z_5\\ Z_1 & Z_6^* & Z_1 & Z_6\\ Z_6^* & Z_5^* & Z_6^* & Z_3+Z_4+2Y_2/v^2\end{pmatrix}. \tag{B9}$$

The massless Goldstone boson eigenvector

$$G^0 = \frac{-i}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\\0\end{pmatrix}, \tag{B10}$$

can be determined by inspection [the normalization factor is chosen for consistency with Eq. (22)]. Thus, we can perform a (unitary) similarity transformation on $\boldsymbol{M}^2$ to remove the Goldstone boson from the neutral Higgs squared-mass matrix. Explicitly, with the unitary matrix

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & -i\\ 0 & 1 & -i & 0\\ 1 & 0 & 0 & i\\ 0 & 1 & i & 0\end{pmatrix}, \tag{B11}$$

it follows from Eq. (B9) that:

$$V^\dagger\boldsymbol{M}^2V = \begin{pmatrix}\mathcal{M} & 0\\ 0 & 0\end{pmatrix}, \tag{B12}$$

where $\mathcal{M}$ is the 3×3 neutral Higgs squared-mass matrix in the $\varphi_1^0 - \varphi_2^0 - a^0$ basis obtained in Eq. (24).

We diagonalize $\mathcal{M}$ as described in Sec. IV. The corresponding diagonalization of $\boldsymbol{M}^2$ is given by

$$\mathcal{D}\boldsymbol{M}^2\mathcal{D}^\dagger \equiv \begin{pmatrix}R & 0\\ 0 & 1\end{pmatrix}V^\dagger\boldsymbol{M}^2V\begin{pmatrix}R^T & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix}\mathcal{M}_D & 0\\ 0 & 0\end{pmatrix}, \tag{B13}$$

where $\mathcal{M}_D = \mathrm{diag}(m_1^2, m_2^2, m_3^2)$ and m_k is the mass of the neutral Higgs mass-eigenstate h_k. The diagonalizing matrix $\mathcal{D}$ is given by

$$\mathcal{D} \equiv \begin{pmatrix}R & 0\\ 0 & 1\end{pmatrix}V^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix}d_{11} & d_{12} & d_{11}^* & d_{12}^*\\ d_{21} & d_{22} & d_{21}^* & d_{22}^*\\ d_{31} & d_{32} & d_{31}^* & d_{32}^*\\ d_{41} & d_{42} & d_{41}^* & d_{42}^*\end{pmatrix}, \tag{B14}$$

where

$$\begin{aligned} d_{11} &= c_{13}c_{12}, & d_{12} &= -s_{123}e^{-i\theta_{23}}, \\ d_{21} &= c_{13}s_{12}, & d_{22} &= c_{123}e^{-i\theta_{23}}, \\ d_{31} &= s_{13}, & d_{32} &= ic_{13}e^{-i\theta_{23}}, \\ d_{41} &= i, & d_{42} &= 0, \end{aligned} \tag{B15}$$

with the c_{ij} and s_{ij} defined in Eq. (28) and

$$c_{123} \equiv c_{12} - is_{12}s_{13}, \qquad s_{123} \equiv s_{12} + ic_{12}s_{13}. \tag{B16}$$

Note that $\mathcal{D}$ is a unitary matrix and $\det\mathcal{D} = 1$. Unitarity implies that

$$\mathrm{Re}\,(d_{k1}d^*_{\ell 1} + d_{k2}d^*_{\ell 2}) = \delta_{k\ell}, \tag{B17}$$

$$\begin{gathered} \frac{1}{2}\sum_{k=1}^{4}|d_{k1}|^2 = \frac{1}{2}\sum_{k=1}^{4}|d_{k2}|^2 = 1, \\ \sum_{k=1}^{4} d_{k2}^2 = \sum_{k=1}^{4} d_{k1}d_{k2} = 0. \end{gathered} \tag{B18}$$

Noting that $d_{41} = i$ and $d_{42} = 0$ [and using Eq. (B22)], these equations reduce to Eqs. (36) and (37) given in Sec. IV. In addition, $\det\mathcal{D} = -i\det RW = 1$, where RW is given in Eq. (33). This yields an additional constraint on the $d_{k\ell}$ [c.f. Eq. (35)].

The matrix $\mathcal{D}$ converts the neutral Higgs basis fields into the neutral Higgs mass-eigenstates:

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ G^0 \end{pmatrix} = \mathcal{D}\begin{pmatrix} \bar{H}_1^{0\dagger} \\ H_2^{0\dagger} \\ \bar{H}_1^0 \\ H_2^0 \end{pmatrix}, \tag{B19}$$

where $\bar{H}_1^0 \equiv H_1^0 - v/\sqrt{2}$.

The mass-eigenstate fields do not depend on the choice of basis. Using the fact that H_1 is invariant and H_2 is pseudoinvariant with respect to flavor-U(2) ransformations, Eq. (B19) implies that the d_{k1} are invariants whereas the d_{k2} are pseudoinvariants with the same transformation law as H_2 [Eq. (20)]. One can also check this directly from Eq. (B13), using the fact that the physical Higgs masses must be basis-independent. These results then imply that θ_{12} and θ_{13} are invariant whereas $e^{i\theta_{23}}$ is a pseudoinvariant, i.e., $e^{i\theta_{23}} \to (\det U)^{-1}e^{i\theta_{23}}$ under an arbitrary flavor-U(2) transformation U.

Finally, using the results of this appendix, we can eliminate the Higgs basis fields entirely and obtain the diagonalizing matrix that converts the neutral Higgs fields in the generic basis into the neutral Higgs mass-eigenstates:

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ G^0 \end{pmatrix} = \mathcal{D}\begin{pmatrix} \bar{\Phi}_{\bar{b}}^{0\dagger}\hat{U}^\dagger_{b\bar{a}} \\ \hat{U}_{a\bar{b}}\bar{\Phi}_b^0 \end{pmatrix}, \tag{B20}$$

where $\bar{\Phi}_a^0 \equiv \Phi_a^0 - v\hat{v}_a/\sqrt{2}$ and $\hat{U}$ is the matrix that converts the generic-basis fields into the Higgs basis fields [see Eq. (10)]. Equation (B20) then yields:

$$h_k = \frac{1}{\sqrt{2}}[\bar{\Phi}_{\bar{a}}^{0\dagger}(d_{k1}\hat{v}_a + d_{k2}\hat{w}_a) + (d^*_{k1}\hat{v}^*_{\bar{a}} + d^*_{k2}\hat{w}^*_{\bar{a}})\bar{\Phi}_a^0], \tag{B21}$$

where $h_4 \equiv G^0$. Note that the U(2)-invariance of the h_k imply that the d_{k1} are invariants and the d_{k2} are pseudoinvariants that transform oppositely to $\hat{w}$ as $d_{k2} \to (\det U)d_{k2}$ in agreement with the previous results above. Indeed, it is useful to define

$$d_{k1} \equiv q_{k1} \quad \text{and} \quad d_{k2} \equiv q_{k2}e^{-i\theta_{23}}, \tag{B22}$$

where *all* the $q_{k\ell}$ are U(2)-invariant [see Eq. (39)]. In particular, $\hat{w}_a e^{-i\theta_{23}}$ is a proper vector with respect to flavor-U(2) transformations. Hence,

$$\begin{aligned} h_k = \frac{1}{\sqrt{2}}[&\bar{\Phi}_{\bar{a}}^{0\dagger}(q_{k1}\hat{v}_a + q_{k2}\hat{w}_a e^{-i\theta_{23}}) \\ &+ (q^*_{k1}\hat{v}^*_{\bar{a}} + q^*_{k2}\hat{w}^*_{\bar{a}}e^{i\theta_{23}})\bar{\Phi}_a^0] \end{aligned} \tag{B23}$$

provides an invariant expression for the neutral Higgs mass-eigenstates.

APPENDIX C: EXPLICIT FORMULAE FOR THE NEUTRAL HIGGS MASSES AND MIXING ANGLES

To obtain expressions for the neutral Higgs masses and mixing angles, we insert Eq. (46) into Eq. (2), and expand out the resulting expression, keeping only terms that are linear and quadratic in the fields. Using Eqs. (17) and (18), one can express the resulting expression in terms of the invariants (Y_1, Y_2, and $Z_{1,2,3,4}$) and pseudoinvariants ($Y_3, Z_{5,6,7}$). The terms linear in the fields vanish if the potential minimum conditions [Eq. (21)] are satisfied. We then eliminate Y_1 and Y_3 from the expressions of the quadratic terms. The result is

$$\begin{aligned} \mathcal{V}_2 = {}& H^+H^-\left(Y_2 + \frac{1}{2}v^2Z_3\right) + \frac{1}{2}v^2h_jh_k\Big\{Z_1\mathrm{Re}(q_{j1})\mathrm{Re}(q_{k1}) \\ &+ \left[\frac{1}{2}(Z_3+Z_4) + Y_2/v^2\right]\mathrm{Re}(q_{j2}q^*_{k2}) \\ &+ \frac{1}{2}\mathrm{Re}(Z_5q_{j2}q_{k2}e^{-2i\theta_{23}}) + \mathrm{Re}(q_{j1})\mathrm{Re}(Z_6q_{k2}e^{-i\theta_{23}}) \\ &+ \mathrm{Re}(q_{k1})\mathrm{Re}(Z_6q_{j2}e^{-i\theta_{23}})\Big\} \\ = {}& m^2_{H^\pm}H^+H^- + \frac{1}{2}\sum_k m_k^2(h_k)^2 + \frac{1}{2}v^2\sum_{j\neq k}C_{jk}h_jh_k, \end{aligned} \tag{C1}$$

where there is an implicit sum over j, $k = 1, \ldots, 4$ (with $h_4 \equiv G^0$). However, since $q_{41} = i$ and $q_{42} = 0$, it is clear that there are no terms in Eq. (C1) involving G^0. Hence, we may restrict the sum to run over j, $k = 1, 2, 3$. The charged Higgs mass obtained above confirms the result quoted in Eq. (23). The neutral Higgs boson masses are given by

$$m_k^2 = |q_{k2}|^2 A^2 + v^2[q_{k1}^2 Z_1 + \mathrm{Re}(q_{k2})\,\mathrm{Re}(q_{k2} Z_5 e^{-2i\theta_{23}}) + 2q_{k1}\,\mathrm{Re}(q_{k2} Z_6 e^{-i\theta_{23}})], \tag{C2}$$

where A^2 is defined in Eq. (42). It is often convenient to assume that $m_1 \leq m_2 \leq m_3$.

Note that the right-hand side of Eq. (C2) is manifestly U(2)-invariant. Moreover, by using Eqs. (36) and (37), one finds that the sum of the three neutral Higgs boson squared-masses is given by

$$\mathrm{Tr}\,\mathcal{M} = \sum_k m_k^2 = 2Y_2 + (Z_1 + Z_3 + Z_4)v^2, \tag{C3}$$

as expected. A more explicit form for the neutral Higgs squared-masses than the one obtained in Eq. (C2) would require the solution of the cubic characteristic equation [Eq. (25)]. Although an analytic solution can be found, it is too complicated to be of much use (a numerical evaluation is more practical).

The coefficients C_{jk} of Eq. (C1) must vanish. Since C_{jk} is symmetric under the interchange of its indices, the conditions $C_{jk} = 0$ yield three independent equations that determine the two mixing angles θ_{12} and θ_{13} and an invariant combination of θ_{23} and the phase of Z_6 (or Z_5). These three invariant angles are defined modulo π once a definite convention is established for the signs of neutral Higgs mass-eigenstate fields (as discussed at the end of section IV). Unique solutions for the invariant angles within this domain are obtained after a mass ordering for the three neutral Higgs bosons is specified (except at certain singular points of the 2HDM parameter space as noted in footnote 8).

To determine explicit formulae for the invariant angles, we shall initially assume that $Z_6 \equiv |Z_6|e^{i\theta_6} \neq 0$ and define the invariant angles ϕ and θ_{56}:

$$\begin{matrix} \phi \equiv \theta_6 - \theta_{23}, \\ \theta_{56} \equiv \theta_5 - \theta_6, \end{matrix} \quad \text{where} \quad \begin{cases} \theta_6 \equiv \arg Z_6, \\ \theta_5 \equiv \frac{1}{2}\arg Z_5. \end{cases} \tag{C4}$$

The factor of $1/2$ in the definition of θ_5 has been inserted for convenience. As discussed in Sec. IV, we can fix the conventions for the overall signs of the h_k fields by restricting the domain of θ_{12}, θ_{13}, and ϕ to the region:

$$-\pi/2 \leq \theta_{12}, \theta_{13} < \pi/2, \qquad 0 \leq \phi < \pi. \tag{C5}$$

One can obtain more tractable equations for θ_{13} and ϕ by taking appropriate linear combinations of the C_{jk}:

$$C_{23}c_{12} - C_{13}s_{12} = s_{13}\,\mathrm{Re}(Z_6 e^{-i\theta_{23}}) - \tfrac{1}{2}c_{13}\,\mathrm{Im}(Z_5 e^{-2i\theta_{23}}), \tag{C6}$$

$$C_{23}s_{12} + C_{13}c_{12} = \tfrac{1}{2}(Z_1 - A^2/v^2)\sin 2\theta_{13} - \cos 2\theta_{13}\,\mathrm{Im}(Z_6 e^{-i\theta_{23}}). \tag{C7}$$

Setting $C_{13} = C_{23} = 0$ yields:

$$\tan\theta_{13} = \frac{\mathrm{Im}(Z_5 e^{-2i\theta_{23}})}{2\,\mathrm{Re}(Z_6 e^{-i\theta_{23}})}, \tag{C8}$$

$$\tan 2\theta_{13} = \frac{2\,\mathrm{Im}(Z_6 e^{-i\theta_{23}})}{Z_1 - A^2/v^2}. \tag{C9}$$

Using the identity $\tan 2\theta_{13} = 2\tan\theta_{13}/(1 - \tan^2\theta_{13})$, one can use Eqs. (C8) and (C9) to eliminate θ_{13} and obtain an equation for ϕ.[22] The resulting equation for ϕ has more than one solution. Plugging a given solution for ϕ back into Eq. (C8) yields a corresponding solution for θ_{13}. Note that if (θ_{13}, ϕ) is a solution to Eqs. (C8) and (C9), then so is $(-\theta_{13}, \phi \pm \pi)$, in agreement with Eqs. (49) and (51). By restricting to the domain of θ_{13} and ϕ specified by Eq. (C5), only one of these two solutions survives. However, multiple solutions to Eqs. (C8) and (C9) still exist within the allowed domain, which correspond to different choices for the mass ordering of the three neutral Higgs fields. By imposing a particular mass ordering, a unique solution is selected [see Eqs. (C21) and (C25)].

Finally, having obtained ϕ and $\tan\theta_{13}$, we use $C_{12} = 0$ to compute θ_{12}. The result is

$$\tan 2\theta_{12} = \frac{s_{13}\,\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) + 2c_{13}\,\mathrm{Re}(Z_6 e^{-i\theta_{23}})}{c_{13}^2(A^2/v^2 - Z_1) + \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) - 2s_{13}c_{13}\,\mathrm{Im}(Z_6 e^{-i\theta_{23}})}. \tag{C10}$$

We can simplify the above result by using Eqs. (C8) and (C9) to solve for $\mathrm{Im}(Z_5 e^{-2i\theta_{23}})$ and $\mathrm{Im}(Z_6 e^{-i\theta_{23}})$ and eliminate these factors from Eq. (C10). The end result is

$$\tan 2\theta_{12} = \frac{2\cos 2\theta_{13}\,\mathrm{Re}(Z_6 e^{-i\theta_{23}})}{c_{13}[c_{13}^2(A^2/v^2 - Z_1) + \cos 2\theta_{13}\,\mathrm{Re}(Z_5 e^{-2i\theta_{23}})]}. \tag{C11}$$

Note that if θ_{12} is a solution to Eq. (C11), then $\theta_{12} \pm \pi/2$ is also a solution. That is, Eq. (C11) yields two solutions for θ_{12} in the allowed domain [Eq. (C5)], which correspond to the two possible mass orderings of h_1 and h_2 as shown below Eq. (C24).

The neutral Higgs boson masses were given in Eq. (C2). With the help of Eqs. (C8), (C9), and (C11), one can can express these masses in terms of Z_1, Z_6, and the invariant angles:

$$m_1^2 = \left[Z_1 - \frac{s_{12}}{c_{12}c_{13}}\,\mathrm{Re}(Z_6 e^{-i\theta_{23}}) + \frac{s_{13}}{c_{13}}\,\mathrm{Im}(Z_6 e^{-i\theta_{23}})\right]v^2, \tag{C12}$$

[22] Recall that the quantity A^2 [Eq. (42)] depends on ϕ via $\mathrm{Re}(Z_5 e^{-2i\theta_{23}}) = |Z_5|\cos 2(\theta_{56} + \phi)$.

$$m_2^2 = \left[Z_1 + \frac{c_{12}}{s_{12}c_{13}} \mathrm{Re}(Z_6 e^{-i\theta_{23}}) + \frac{s_{13}}{c_{13}} \mathrm{Im}(Z_6 e^{-i\theta_{23}}) \right] v^2, \tag{C13}$$

$$m_3^2 = \left[Z_1 - \frac{c_{13}}{s_{13}} \mathrm{Im}(Z_6 e^{-i\theta_{23}}) \right] v^2. \tag{C14}$$

For the subsequent analysis, it is useful to invert Eqs. (C12)–(C14) and solve for Z_1, $\mathrm{Re}(Z_6 e^{-i\theta_{23}})$, and $\mathrm{Im}(Z_6 e^{-i\theta_{23}})$:

$$Z_1 v^2 = m_1^2 c_{12}^2 c_{13}^2 + m_2^2 s_{12}^2 c_{13}^2 + m_3^2 s_{13}^2, \tag{C15}$$

$$\mathrm{Re}\,(Z_6 e^{-i\theta_{23}}) v^2 = c_{13} s_{12} c_{12} (m_2^2 - m_1^2), \tag{C16}$$

$$\mathrm{Im}\,(Z_6 e^{-i\theta_{23}}) v^2 = s_{13} c_{13} (c_{12}^2 m_1^2 + s_{12}^2 m_2^2 - m_3^2). \tag{C17}$$

In addition, Eqs. (C9) and (C11) can be used to express $\mathrm{Re}(Z_5 e^{-i\theta_{23}})$ in terms of Z_6:

$$\mathrm{Re}\,(Z_5 e^{-2i\theta_{23}}) = \frac{c_{13}}{s_{13}} \mathrm{Im}(Z_6 e^{-i\theta_{23}}) + \frac{c_{12}^2 - s_{12}^2}{c_{13} s_{12} c_{12}} \mathrm{Re}(Z_6 e^{-i\theta_{23}}). \tag{C18}$$

Inserting Eqs. (C16) and (C17) into Eqs. (C8) and (C18) then yields expressions for $\mathrm{Im}(Z_5 e^{-i\theta_{23}})$ and $\mathrm{Re}(Z_5 e^{-i\theta_{23}})$ in terms of the invariant angles and the neutral Higgs masses.

The above results can be used to derive an expression for

$$\begin{aligned} \mathrm{Im}(Z_5^* Z_6^2) = {} & 2\,\mathrm{Re}(Z_5 e^{-2i\theta_{23}})\,\mathrm{Re}(Z_6 e^{-i\theta_{23}})\,\mathrm{Im}(Z_6 e^{-i\theta_{23}}) \\ & - \mathrm{Im}(Z_5 e^{-2i\theta_{23}})[\mathrm{Re}(Z_6 e^{-i\theta_{23}})]^2 \\ & + \mathrm{Im}(Z_5 e^{-2i\theta_{23}})[\mathrm{Im}(Z_6 e^{-i\theta_{23}})]^2. \end{aligned} \tag{C19}$$

Using Eqs. (C8) and (C16)–(C18), one can simplify the right-hand side of Eq. (C19) to obtain:

$$\begin{aligned} \mathrm{Im}(Z_5^* Z_6^2) v^6 = {} & 2 s_{13} c_{13}^2 s_{12} c_{12} (m_2^2 - m_1^2)(m_3^2 - m_1^2) \\ & \times (m_3^2 - m_2^2). \end{aligned} \tag{C20}$$

Equation (C20) was first derived in Ref. [21]; it is equivalent to a result initially obtained in Ref. [45]. In particular, if any two of the neutral Higgs masses are degenerate, then $\mathrm{Im}(Z_5^* Z_6^2) = 0$, in which case one can always find a basis in which the pseudoinvariants Z_5 and Z_6 are simultaneously real. The neutral scalar squared-mass matrix [Eq. (24)] then breaks up into a block diagonal form consisting of a 2×2 block and a 1×1 block. The diagonalization of the 2×2 block has a simple analytic form, and the neutral scalar mixing can be treated more simply by introducing one invariant mixing angle instead of the three needed in the general case. Note that $\mathrm{Im}(Z_5^* Z_6^2) = 0$ is a necessary (although not sufficient) requirement for a *CP*-conserving Higgs sector, as discussed in Appendix D. For the remainder of this appendix, we shall assume that the neutral Higgs boson masses are nondegenerate.

In order to facilitate the discussion of the *CP*-conserving limit and the decoupling limit of the 2HDM (which are treated in Appendix D), it is useful to derive a number of additional relations for the invariant angles. First, we employ Eqs. (C12)–(C14) to eliminate θ_{12} and ϕ and obtain a single equation for θ_{13}:

$$s_{13}^2 = \frac{(Z_1 v^2 - m_1^2)(Z_1 v^2 - m_2^2) + |Z_6|^2 v^4}{(m_3^2 - m_1^2)(m_3^2 - m_2^2)}. \tag{C21}$$

Equation (C21) determines c_{13} (in the convention where $c_{13} \geq 0$). The sign of s_{13} is determined from Eq. (C14), which can be rewritten as

$$\sin\phi = \frac{(Z_1 v^2 - m_3^2)\tan\theta_{13}}{|Z_6| v^2}. \tag{C22}$$

Since $\sin\phi \geq 0$ in the angular domain specified by Eq. (C5), it follows that the sign of s_{13} is equal to the sign of $Z_1 v^2 - m_3^2$. In particular, if m_3^2 is the largest eigenvalue of $\tilde{\mathcal{M}}$ [Eq. (24)], then it must be greater than the largest diagonal element of $\tilde{\mathcal{M}}$. That is, $Z_1 v^2 - m_3^2 < 0$ if $m_3 > m_{1,2}$, in which case $s_{13} \leq 0$.

However, Eq. (C22) does not fix the sign of $\cos\phi$. To determine this sign, we can use Eq. (C8) to eliminate θ_{13} from Eq. (C22). Consequently, one obtains a single equation for ϕ:

$$\tan 2\phi = \frac{\mathrm{Im}(Z_5^* Z_6^2)}{\mathrm{Re}(Z_5^* Z_6^2) + [(|Z_6|^4 v^2)/(m_3^2 - Z_1 v^2)]}. \tag{C23}$$

Given $\sin\phi \geq 0$ and $\tan 2\phi$ in the region $0 \leq \phi < \pi$, one can uniquely determine ϕ (and hence the sign of $\cos\phi$). Thus, for a fixed ordering of the neutral Higgs masses, Eqs. (C21)–(C23) provide a unique solution for (θ_{13}, ϕ) in the domain $-\pi/2 \leq \theta_{13} < \pi/2$ and $0 \leq \phi < \pi$.

Next, we note that Eq. (C16) can be rewritten as

$$\sin 2\theta_{12} = \frac{2|Z_6| v^2 \cos\phi}{c_{13}(m_2^2 - m_1^2)}. \tag{C24}$$

As advertised below Eq. (C11), the mass ordering of m_1 and m_2 fixes the sign of $\sin 2\theta_{12}$. In particular, in the angular domain of Eq. (C5), $m_2 > m_1$ implies that $s_{12}\cos\phi \geq 0$. The sign of s_{12} is fixed after using Eq. (C20) to infer that $\sin 2\theta_{56}\cos\phi \geq 0$ for $m_3 > m_2 > m_1$.

An alternative expression for θ_{12} can be obtained by combining Eqs. (C15) and (C21), which yields

$$c_{13}^2 s_{12}^2 = \frac{(Z_1 v^2 - m_1^2)(m_3^2 - Z_1 v^2) - |Z_6|^2 v^4}{(m_2^2 - m_1^2)(m_3^2 - m_2^2)}. \tag{C25}$$

Note the similarity of the expressions given by Eqs. (C21) and (C25); both these results play an important role in determining the conditions that govern the decoupling limit.

A simpler form for $\tan^2\theta_{13}$ can also be obtained by combining Eqs. (C9) and (C22):

$$\tan^2\theta_{13} = \frac{m_3^2 - A^2}{m_3^2 - Z_1 v^2}. \tag{C26}$$

Finally, one can derive an expression for $m_2^2 - m_3^2$, after eliminating $\mathrm{Im}(Z_6 e^{-i\theta_{23}})$ in favor of $\mathrm{Re}(Z_5 e^{-2i\theta_{23}})$ using Eq. (C18):

$$m_2^2 - m_3^2 = \frac{v^2}{c_{13}^2}\left[\mathrm{Re}(Z_5 e^{-2i\theta_{23}}) + \frac{c_{13}(s_{12}^2 - c_{12}^2 s_{13}^2)}{s_{12}c_{12}}\mathrm{Re}(Z_6 e^{-i\theta_{23}})\right]. \tag{C27}$$

The expressions for the differences of squared-masses [Eqs. (C24) and (C27)] take on rather simple forms in the CP-conserving limit.

For completeness, we end this appendix with a treatment of the case where $Z_6 = 0$. Since all three neutral Higgs squared-masses are assumed to be nondegenerate, we require that $Z_5 \equiv |Z_5|e^{2i\theta_5} \neq 0$ in what follows,[23] and define the invariant angle $\phi_5 \equiv \theta_5 - \theta_{23}$. Once the sign conventions of the neutral Higgs fields are fixed, the invariant angles θ_{12}, θ_{13}, and ϕ_5 are defined modulo π. We first note that Eqs. (C6), (C7), and (C10) are valid when $Z_6 = 0$. Thus, setting Eq. (C7) to zero implies that $\sin 2\theta_{13} = 0$,[24] which yields two possible cases: (i) $s_{13} = 0$ or (ii) $c_{13} = 0$.

If (i) $s_{13} = 0$, then Eq. (C6) yields $\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$, i.e., $\sin 2\phi_5 = 0$, and Eq. (C10) implies that $\sin 2\theta_{12} = 0$. Thus, we obtain four possible solutions for the invariant angles modulo π, which correspond to four of the possible six mass orderings of the three neutral Higgs states. If (ii) $c_{13} = 0$ [and $s_{13} = -1$ in the convention of Eq. (C5)], then Eq. (C10) implies that $\tan 2\theta_{12} = -\tan 2\phi_5$, or equivalently $\sin 2(\theta_{12} + \phi_5) = \sin 2(\theta_{12} - \theta_{23} + \theta_5) = 0$. In particular, in a basis in which Z_5 is real, the rotation matrix R [Eq. (28)] depends only on the combination $\theta_{12} - \theta_{23}$ when $s_{13} = -1$ (so that $\theta_{12} + \theta_{23}$ is indeterminate). Note that $q_{31} = -1$, $q_{41} = i$, $q_{22} = -iq_{12} = e^{i\theta_{12}}$, and $q_{11} = q_{21} = q_{32} = q_{42} = 0$. Indeed, only the combination $\theta_{12} - \theta_{23}$ enters the Higgs couplings in a real Z_5 basis. Consequently, the condition $\sin 2(\theta_{12} + \phi_5) = 0$ yields two solutions modulo π, which correspond to the final two possible mass orderings of the neutral Higgs states.

[23] If $Z_5 = Z_6 = 0$, then the neutral Higgs squared-mass matrix is diagonal in the Higgs basis, with two degenerate Higgs boson mass-eigenstates.

[24] If $Z_6 = 0$ and $A^2 = Z_1 v^2$, then Eq. (C7) is automatically equal to zero. In this we set Eq. (C6) to zero and conclude that either $c_{13} = 0$ or $\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$. If the latter holds true, then the squared-mass matrix $\tilde{\mathcal{M}}$ [see Eq. (41)] is diagonal with degenerate eigenvalues.

APPENDIX D: THE CP-CONSERVING AND THE DECOUPLING LIMITS OF THE 2HDM

To make contact with the 2HDM literature, we consider two limiting cases of the most general 2HDM—the CP-conserving limit and the decoupling limit.

1. The CP-conserving limit of the 2HDM

In the CP-conserving limit, we impose CP-invariance on all bosonic couplings and fermionic couplings of the Higgs bosons. The requirement of a CP-conserving bosonic sector is equivalent to the requirement that the scalar potential is explicitly CP-conserving and that the Higgs vacuum is CP-invariant (i.e., there is no spontaneous CP-violation). Basis-independent conditions for a CP-conserving bosonic sector have been given in Refs. [17,18,21,22]. In Ref. [17], these conditions were recast into the following form. The bosonic sector is CP-conserving if and only if[25]:

$$\mathrm{Im}[Z_6 Z_7^*] = \mathrm{Im}[Z_5^* Z_6^2] = \mathrm{Im}[Z_5^*(Z_6 + Z_7)^2] = 0. \tag{D1}$$

Equation (D1) is equivalent to the requirement that

$$\sin 2(\theta_5 - \theta_6) = \sin 2(\theta_5 - \theta_7) = \sin(\theta_6 - \theta_7) = 0, \tag{D2}$$

where θ_5 and θ_6 are defined in Eq. (C4) and $\theta_7 \equiv \arg Z_7$ (note that θ_5 is defined modulo π and θ_6 and θ_7 are defined modulo 2π).

Additional constraints arise when the Higgs-fermion couplings are included. Consider the most general coupling of the two Higgs doublets to three generations of quarks and leptons, as described in section VI. As we shall demonstrate below Eq. (D21), if

$$Z_5[\rho^Q]^2, \quad Z_6\rho^Q \quad \text{and} \quad Z_7\rho^Q \text{ are Hermitian matrices} \quad (Q = U, D, E), \tag{D3}$$

then the couplings of the neutral Higgs bosons to fermion pairs are CP-invariant. Thus, if Eqs. (D1) and (D3) are satisfied, then the neutral Higgs bosons are eigenstates of CP, and the only possible source of CP-violation in the 2HDM is the unremovable phase in the CKM matrix K that enters via the charged current interactions mediated by either $W^\pm$ or $H^\pm$ exchange[26] [see Eq. (82)].

[25] Since the scalar potential minimum conditions imply that $Y_3 = -\frac{1}{2}Z_6 v^2$, no separate condition involving Y_3 is required.

[26] One can also formulate a basis-independent condition (that is invariant with respect to separate redefinitions of the Higgs-doublet fields and the quark fields) for the absence of CP-violation in the charged current interactions. This condition involves the Jarlskog invariant [46], and can also be written as [7,47]: $\mathrm{Tr}_f[H^{U,0}, H^{D,0}]^3 = 0$ (summed over three quark generations), where $H^{Q,0} \equiv M^{Q,0}M^{Q,0\dagger}$ and the $M^{Q,0}$ are defined below Eq. (81). Since CP-violating phenomena in the charged current interactions are observed and well described by the CKM matrix, we shall not impose this latter condition here.

One can explore the consequences of CP-invariance by studying the pattern of Higgs couplings and the structure of the neutral Higgs boson squared-mass matrix [Eq. (24)]. Note that the tree-level couplings of G^0 are CP-conserving, even in the general CP-violating 2HDM. In particular, the couplings $G^0G^0G^0$, $G^0G^+G^-$, $G^0H^+H^-$, and ZZG^0 are absent. Moreover, Eq. (83) implies that G^0 possesses purely pseudoscalar couplings to the fermions. Hence, G^0 is a CP-odd scalar, independently of the structure of the scalar potential. We can therefore use the couplings of G^0 to the neutral Higgs bosons as a probe of the CP-quantum numbers of these states. The analysis of the neutral Higgs boson squared-mass matrix (which does not depend on Z_7) simplifies significantly when $\mathrm{Im}[Z_5^*Z_6^2] = 0$. One can then choose a basis where Z_5 and Z_6 are simultaneously real, in which case the scalar squared-mass matrix decomposes into diagonal block form. The upper 2×2 block can be diagonalized analytically and yields the mass-eigenstates h^0 and H^0 (with $m_{h^0} \le m_{H^0}$). The lower 1×1 block yields the mass-eigenstate A^0. If all the conditions of Eqs. (D1) and (D3) are satisfied, then the neutral Higgs boson mass-eigenstates are also states of definite CP quantum number. We shall demonstrate below that h^0 and H^0 are CP-even scalars and A^0 is a CP-odd scalar.

We first consider the special case of $Z_6 = 0$. In this case, the scalar squared-mass matrix is diagonal in a basis where Z_5 is real. It is convenient to choose $c_{12} = c_{13} = c_{23} = 1$ (corresponding to one of the possible Higgs mass orderings, as discussed at the end of Appendix C). For this choice of invariant mixing angles, $q_{11} = q_{22} = 1$, $q_{41} = q_{32} = i$, and all other $q_{k\ell}$ vanish. These results then fix all the Higgs couplings. The existence of nonzero ZG^0h_1 and Zh_2h_3 couplings imply that h_1 is CP-even, and h_2 and h_3 are states of opposite CP quantum number. If Eqs. (D1) and (D3) hold with $Z_7 \neq 0$ and/or $\rho^Q \neq 0$, then one can use the nonzero $H^+H^-h_2$ and/or the $\bar{Q}Qh_2$ couplings to conclude that h_2 is CP-even and h_3 is CP-odd. Thus, we can identify[27] $h_3 = A^0$ and $h_{1,2} = h^0, H^0$ (the mass ordering of the latter two states is not yet determined). The scalar squared masses [Eq. (43)] are given by:

$$m_1^2 = Z_1 v^2, \qquad m_{2,3}^2 = Y_2 + \tfrac{1}{2}[Z_3 + Z_4 \pm \varepsilon|Z_5|]v^2, \quad \text{(D4)}$$

where $\varepsilon \equiv \cos 2(\theta_5 - \theta_{23}) = \pm 1$. In general, these scalar squared-masses will not satisfy $m_1 \le m_2 \le m_3$. In a real Z_5 basis with $\theta_{23} = 0$, it follows that $\varepsilon|Z_5| = Z_5$. For example, if $m_1 \le m_2$ (in which case, $h_1 = h^0$ and $h_2 = H^0$), then $m_{H^0}^2 - m_{A^0}^2 = Z_5 v^2$. A different choice for the θ_{ij} can be made to reorder the neutral Higgs states in ascending mass order.

If $\mathrm{Im}(Z_5^*Z_6^2) = 0$ and $Z_6 \neq 0$, one possible choice is $c_{13} = c_{23} = 1$ (in a basis where Z_5 and Z_6 are real), in which case θ_{12} is determined by diagonalizing the upper left 2×2 block of Eq. (24). However, it is instructive to consider the implications of the more general results of Appendix C. Since $Z_6 \neq 0$ by assumption, Eq. (C23) yields $\sin\phi\cos\phi = 0$, and Eq. (C20) implies that either some of the neutral Higgs boson masses are degenerate or $s_{13}s_{12}c_{12} = 0$.[28] In the case of degenerate masses, some of the invariant angles are not well defined, since any linear combination of the degenerate states is also a mass-eigenstate. Hence, the degenerate case must be treated separately. In what follows, we shall assume that all three neutral Higgs boson masses are nondegenerate. Note that if $\sin\phi = 0$, then Eq. (C22) yields $s_{13} = 0$, whereas if $\cos\phi = 0$, then Eq. (C24) yields $\sin 2\theta_{12} = 0$.[29] Thus, we shall consider separately the two cases: (I) $s_{13} = \sin\phi = 0$ and (II) $\cos\phi = \sin 2\theta_{12} = 0$.

Consider Case I where $s_{13} = \sin\phi = 0$. With the angles restricted as specified in Eq. (C5),

$$\theta_{13} = 0, \qquad \phi = 0, \qquad [\text{Case I}]. \qquad \text{(D5)}$$

Next, we examine Case II where $\cos\phi = \sin 2\theta_{12} = 0$. It is convenient to consider separately two subcases: (IIa) $s_{12} = \cos\phi = 0$ and (IIb) $c_{12} = \cos\phi = 0$. More explicitly,

$$\theta_{12} = 0, \qquad \phi = \tfrac{1}{2}\pi, \qquad [\text{Case IIa}], \qquad \text{(D6)}$$

$$\theta_{12} = -\tfrac{1}{2}\pi, \qquad \phi = \tfrac{1}{2}\pi, \qquad [\text{Case IIb}]. \qquad \text{(D7)}$$

The values of the $q_{k\ell}$ corresponding to cases I, IIa and IIb are given in Tables II, III, and IV.

Using these values of the $q_{k\ell}$ [along with the values of ϕ given in Eqs. (D5)–(D7)], we can employ the bosonic couplings of the Higgs bosons to determine the CP-quantum numbers of the three neutral states, h_k. Using the same techniques as in the $Z_6 = 0$ case treated previously, we again conclude that one of the three neutral Higgs states is CP-odd and the other two are CP-even. The existence of three cases [I, IIa, and IIb above] corresponds to the three possible neutral Higgs fields that can be identified as the CP-odd scalar. The three cases can also be understood from the structure of the matrix $\tilde{\mathcal{M}}$ given in Eq. (41). In particular, if $\mathrm{Im}(Z_5^*Z_6^2) = 0$ and $Z_6 \neq 0$, then two possible cases exist:

[27] If $Z_6 = Z_7 = \rho^Q = 0$, then only the relative CP quantum numbers of h_2 and h_3 are well defined.

[28] Since $Z_6 \neq 0$, one can use Eqs. (C8) and (C9) to show that $c_{13} \neq 0$.

[29] The same constraints are obtained by imposing the requirement of CP-conserving Higgs couplings. In particular, the existence of a $G^0h_kh_k$ coupling would imply that h_k is a state of mixed CP-even and CP-odd components. All such couplings must therefore be absent in the CP-conserving limit. Using the results of Eqs. (58) and (D2) one can easily check that at least one of these CP-violating couplings is present unless $s_{13} = \sin\phi = 0$ or $\cos\phi = \sin 2\theta_{12} = 0$.

TABLE II. The U(2)-invariant quantities $q_{k\ell}$ in the CP-conserving limit. Case I: $s_{13}=0$ and $\sin(\theta_6-\theta_{23})=0$. In the standard notation of the CP-conserving 2HDM (with real scalar potential parameters), $e^{-i\theta_{23}}=\mathrm{sgn}Z_6\equiv\varepsilon_6$, which implies that the neutral Higgs fields are $h_1=h^0$, $h_2=-\varepsilon_6 H^0$, $h_3=\varepsilon_6 A^0$, and $h_4=G^0$, and the angular factors are $c_{12}=s_{\beta-\alpha}$ and $s_{12}=-\varepsilon_6 c_{\beta-\alpha}$.

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

TABLE III. The U(2)-invariant quantities $q_{k\ell}$ in the CP-conserving limit. Case IIa: $s_{12}=0$ and $\cos(\theta_6-\theta_{23})=0$. In the standard notation of the CP-conserving 2HDM (with real scalar potential parameters), $e^{-i\theta_{23}}=i\,\mathrm{sgn}Z_6\equiv i\varepsilon_6$, which implies that the neutral Higgs fields are $h_1=h^0$, $h_2=\varepsilon_6 A^0$, $h_3=\varepsilon_6 H^0$, and $h_4=G^0$, and the angular factors are $c_{13}=s_{\beta-\alpha}$ and $s_{13}=\varepsilon_6 c_{\beta-\alpha}$.

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

TABLE IV. The U(2)-invariant quantities $q_{k\ell}$ in the CP-conserving limit. Case IIb: $c_{12}=0$ and $\cos(\theta_6-\theta_{23})=0$. In the standard notation of the CP-conserving 2HDM (with real scalar potential parameters), $e^{-i\theta_{23}}=i\mathrm{sgn}Z_6\equiv i\varepsilon_6$, which implies that the neutral Higgs fields are $h_1=\varepsilon_6 A^0$, $h_2=-h^0$, $h_3=\varepsilon_6 H^0$, and $h_4=G^0$, and the angular factors are $c_{13}=s_{\beta-\alpha}$ and $s_{13}=\varepsilon_6 c_{\beta-\alpha}$.

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

$$\text{Case I:}\quad \sin\phi=0\Rightarrow \mathrm{Im}(Z_5e^{-2i\theta_{23}})=\mathrm{Im}(Z_6e^{-i\theta_{23}})=0, \tag{D8}$$

$$\text{Case II:}\quad \cos\phi=0\Rightarrow \mathrm{Im}(Z_5e^{-2i\theta_{23}})=\mathrm{Re}(Z_6e^{-i\theta_{23}})=0. \tag{D9}$$

In both Case I and Case II, $\tilde{\mathcal{M}}$ assumes a block diagonal form consisting of a 2×2 block (corresponding to the CP-even Higgs bosons) and a 1×1 block (corresponding to the CP-odd Higgs boson). In Case I, the 1×1 block associated with A^0 is the 33 element of $\tilde{\mathcal{M}}$. Thus, $s_{13}=0$ and we identify h_3 as the CP-odd Higgs boson, with mass:

$$m_{A^0}^2=A^2=Y_2+\tfrac{1}{2}v^2[Z_3+Z_4-\mathrm{Re}(Z_5e^{-2i\theta_{23}})] \quad [\text{Case I}]. \tag{D10}$$

In Case IIa, the 1×1 block associated with A^0 is the 22 element of $\tilde{\mathcal{M}}$. Thus, $\theta_{12}=0$, and we identify h_2 as the CP-odd Higgs boson, with mass:

$$\begin{aligned} m_{A^0}^2 &= A^2+v^2\,\mathrm{Re}(Z_5e^{-2i\theta_{23}})\\ &= Y_2+\tfrac{1}{2}v^2[Z_3+Z_4+\mathrm{Re}(Z_5e^{-2i\theta_{23}})] \end{aligned} \quad [\text{Case II}]. \tag{D11}$$

If we choose $\theta_{12}=-\pi/2$ instead of $\theta_{12}=0$ above, then this corresponds to an additional orthogonal transformation $\tilde{\mathcal{M}}\to R_{12}\tilde{\mathcal{M}}R_{12}^T$, where R_{12} is defined in Eq. (28). One can easily check that $R_{12}\tilde{\mathcal{M}}R_{12}^T$ is also in block diagonal matrix form, consisting of a 2×2 block and a 1×1 block. The latter, associated with the CP-odd scalar state, is the 11 element of $R_{12}\tilde{\mathcal{M}}R_{12}^T$. This is Case IIb, and we identify h_1 as the CP-odd Higgs boson, with mass given by Eq. (D11). Note that Eqs. (D5)–(D7) imply that the value of $Z_5e^{-2i\theta_{23}}$ in Case II has the opposite sign from the corresponding result in Case I. Thus, Eqs. (D10) and (D11) yield the same result for the mass of the CP-odd scalar in terms of the model parameters.

In the standard notation of the CP-conserving 2HDM, one considers only real-basis choices, in which the Higgs Lagrangian parameters and the scalar vacuum expectation values are real. We can therefore restrict basis changes to O(2) transformations [17].[30] In this context, pseudoinvariants are SO(2)-invariant quantities that change sign under an O(2) transformation with determinant equal to -1. Note that Z_5 is now an invariant with respect to O(2) transformations, but Z_6, Z_7, and $e^{-i\theta_{23}}$ are pseudoinvariants. In particular, for $Z_6\neq0$ in the convention where $0\le\phi<\pi$,

$$e^{-i\theta_{23}}=e^{i\phi}e^{-i\theta_6}=\begin{cases}\varepsilon_6 & [\text{Case I}],\\ i\varepsilon_6 & [\text{Case II}],\end{cases} \tag{D12}$$

where $Z_6\equiv\varepsilon_6|Z_6|$ in the real basis. That is, ε_6 is a pseudoinvariant quantity (in contrast, the sign of Z_5 is invariant) with respect to O(2) transformations. Using Eq. (D12) in either Eq. (D10) or Eq. (D11) yields m_{A^0} in terms of the real-basis parameters:

$$m_{A^0}^2=Y_2+\tfrac{1}{2}v^2(Z_3+Z_4-Z_5). \tag{D13}$$

The generic real-basis fields can be expressed in terms of the two neutral CP-even scalar mass-eigenstates h^0, H^0 (with $m_{h^0}\le m_{H^0}$) and the CP-odd scalar mass-eigenstate

[30] If $Z_6=Z_7=\rho^Q=0$, then the possible transformations among real bases are elements of $\mathrm{O}(2)\times\mathbb{Z}_2$. In particular, the sign of Z_5 changes when the Higgs basis field $H_2\to iH_2$. In this case, Z_5 is an O(2)-invariant but it is a pseudoinvariant with respect to $\mathbb{Z}_2$.

A^0, G^0 as follows [4,5]:

$$\Phi_1^0 = \frac{1}{\sqrt{2}}[v\hat{v}_1 - h^0 s_\alpha + H^0 c_\alpha + i(G^0 c_\beta - A^0 s_\beta)], \quad \text{(D14)}$$

$$\Phi_2^0 = \frac{1}{\sqrt{2}}[v\hat{v}_2 + h^0 c_\alpha + H^0 s_\alpha + i(G^0 s_\beta + A^0 c_\beta)], \quad \text{(D15)}$$

with $m_{h^0} \le m_{H^0}$, where $\hat{v}_a = (c_\beta, s_\beta)$, $s_\alpha \equiv \sin\alpha$, $c_\alpha \equiv \cos\alpha$, and α is the CP-even neutral Higgs boson mixing angle. These equations can be written more compactly as

$$\Phi_a^0 = \frac{1}{\sqrt{2}}[(v + h^0 s_{\beta-\alpha} + H^0 c_{\beta-\alpha} + iG^0)\hat{v}_a + (h^0 c_{\beta-\alpha} - H^0 s_{\beta-\alpha} + iA^0)\hat{w}_a], \quad \text{(D16)}$$

where $s_{\beta-\alpha} \equiv \sin(\beta - \alpha)$ and $c_{\beta-\alpha} \equiv \cos(\beta - \alpha)$.

Using the results of Tables II, III, and IV and comparing Eq. (D16) to Eq. (46) [with $e^{-i\theta_{23}}$ determined from Eq. (D12)], one can identify the neutral Higgs fields h_k with the eigenstates of definite CP quantum numbers, h^0, H^0, and A^0, and relate the angular factor $\beta - \alpha$ with the appropriate invariant angle[31]:

$$\begin{aligned}
&\text{Case I: } h_1 = h^0, \quad h_2 = -\varepsilon_6 H^0 \quad \text{and} \quad h_3 = \varepsilon_6 A^0,\\
&\qquad c_{12} = s_{\beta-\alpha} \quad \text{and} \quad s_{12} = -\varepsilon_6 c_{\beta-\alpha},\\
&\text{Case IIa: } h_1 = h^0, \quad h_2 = \varepsilon_6 A^0 \quad \text{and} \quad h_3 = \varepsilon_6 H^0,\\
&\qquad c_{13} = s_{\beta-\alpha} \quad \text{and} \quad s_{13} = \varepsilon_6 c_{\beta-\alpha},\\
&\text{Case IIb: } h_1 = \varepsilon_6 A^0, h_2 = -h^0 \quad \text{and} \quad h_3 = \varepsilon_6 H^0,\\
&\qquad c_{13} = s_{\beta-\alpha} \quad \text{and} \quad s_{13} = \varepsilon_6 c_{\beta-\alpha}.
\end{aligned} \quad \text{(D17)}$$

In the convention for the angular domain given by Eq. (C5), c_{12} and c_{13} are non-negative and therefore $s_{\beta-\alpha} \ge 0$. The appearance of the pseudoinvariant quantity ε_6 in Eq. (D17) implies that H^0, A^0 (and $H^\pm$) are pseudoinvariant fields, and $c_{\beta-\alpha}$ is a pseudoinvariant with respect to O(2) transformations.[32] In contrast, h^0 is an invariant field.

At this stage, we have not imposed any mass ordering of the three neutral scalar states. Since one can distinguish between the CP-odd and the CP-even neutral scalars, it is sufficient to require that $m_{h^0} \le m_{H^0}$. (If one does not care about the mass ordering of A^0 relative to the CP-even states, then Cases IIa and IIb can be discarded without loss of generality.) We can compute the masses of the CP-even scalars and the angle $\beta - \alpha$ [43] in any of the three cases:

$$m_{h^0}^2 = m_{A^0}^2 c_{\beta-\alpha}^2 + v^2[Z_1 s_{\beta-\alpha}^2 + Z_5 c_{\beta-\alpha}^2 + 2 s_{\beta-\alpha} c_{\beta-\alpha} Z_6], \quad \text{(D18)}$$

$$m_{H^0}^2 = m_{A^0}^2 s_{\beta-\alpha}^2 + v^2[Z_1 c_{\beta-\alpha}^2 + Z_5 s_{\beta-\alpha}^2 - 2 s_{\beta-\alpha} c_{\beta-\alpha} Z_6], \quad \text{(D19)}$$

and

$$\begin{aligned}
\tan[2(\beta-\alpha)] &= \frac{2Z_6 v^2}{m_{A^0}^2 + (Z_5 - Z_1)v^2},\\
\sin[2(\beta-\alpha)] &= \frac{-2Z_6 v^2}{m_{H^0}^2 - m_{h^0}^2}.
\end{aligned} \quad \text{(D20)}$$

Note that Eqs. (D18)–(D20) are covariant with respect to O(2) transformations, since Z_6 and $c_{\beta-\alpha}$ are both pseudoinvariant quantities.

Additional constraints arise by requiring that the neutral Higgs-fermion couplings are CP-invariant, as previously noted in Eq. (D3). To derive this latter result, we employ the possible values of the $q_{k\ell}$ given in Tables II, III, and IV in the Higgs-fermion interactions given by Eq. (82). In particular, we demand that the couplings of h^0 and H^0 to fermions are scalar interactions, whereas the couplings of A^0 to fermions are pseudoscalar interactions. These requirements produce the following basis-independent conditions:

$$e^{i\theta_{23}}\rho^Q \text{ is } \begin{cases} \text{Hermitian} & \text{in Case I,} \\ \text{anti-Hermitian} & \text{in Cases IIa and IIb.} \end{cases} \quad \text{(D21)}$$

In both Cases I and II, the results of Eqs. (D8), (D9), and (D21) imply that $Z_6\rho^Q = (Z_6 e^{-i\theta_{23}})(e^{i\theta_{23}}\rho^Q)$ is Hermitian. Combining this result with Eq. (D1) then yields Eq. (D3).

Invariant techniques for describing the constraints on the Higgs-fermion interaction due to CP-invariance have also been considered in Refs. [7,22]. In these works, the authors construct invariant expressions that are both U(2)-invariant and invariant with respect to the redefinition of the quark fields. For example, the invariants denoted by J_a and J_b in Ref. [22] are given by $J_a \equiv \mathrm{Im} J^D$ and $J_b \equiv \mathrm{Im} J^U$, where

$$\begin{aligned}
J^Q &= \mathrm{Tr}(VYT^Q),\\
T^Q_{a\bar{b}} &\equiv \mathrm{Tr}_f(\eta_a^{Q,0}\eta_{\bar{b}}^{Q,0\dagger}) = \mathrm{Tr}_f(\eta_a^Q \eta_{\bar{b}}^{Q\dagger}),
\end{aligned} \quad \text{(D22)}$$

and the trace Tr_f sums over the diagonal quark generation indices. Note that the trace over generation indices ensures that the resulting expression is invariant with respect to unitary redefinitions of the quark fields [Eq. (73)]. Using Eq. (B5) [with $A = Y$], it is straightforward to reexpress Eq. (D22) as

$$J^Q = Y_1 \mathrm{Tr}_f[(\kappa^Q)^2] + Y_3 \mathrm{Tr}_f[\kappa^Q \rho^Q], \quad \text{(D23)}$$

after using Eqs. (17), (18), and (77). Indeed, J^Q is invariant with respect to U(2) transformations since the product of

[31] The extra minus signs in the identification of $h_2 = -\varepsilon_6 H^0$ in Case I and $h_2 = -h^0$ in Case IIb arise due to the fact that the standard conventions of the CP-conserving 2HDM correspond to $\det R = -1$ (whereas $\det R = +1$ in Case IIa).

[32] Note that $s_{\beta-\alpha}$ is invariant with respect to O(2) transformations, which is consistent with our convention that $s_{\beta-\alpha} \ge 0$. The analogous results have been obtained in Ref. [17] in a convention where $c_{\beta-\alpha} \ge 0$.

pseudoinvariants $Y_3\rho^Q$ is a U(2)-invariant quantity. Moreover, taking the trace over the quark generation indices ensures that J^Q is invariant with respect to unitary redefinitions of the quark fields. In Ref. [22], a proof is given that $\mathrm{Im}J^Q = 0$ is one of the invariant conditions for CP-invariance of the Higgs-fermion interactions. In our formalism, this result is easily verified. Using the scalar potential minimum conditions [Eq. (21)], we obtain:

$$\mathrm{Im}\, J^Q = -\frac{v}{\sqrt{2}}\,\mathrm{Im}[Z_6\,\mathrm{Tr}_f(M_Q\rho^Q)]. \tag{D24}$$

But, CP-invariance requires [by Eq. (D3)] that $Z_6\rho^Q$ is hermitian. Since M_Q is a real diagonal matrix, it then immediately follows that $\mathrm{Im}J^Q = 0$.

We end this subsection with a very brief outline of the tree-level MSSM Higgs sector. Since this model is CP-conserving, it is conventional to choose the phase conventions of the Higgs fields that yield a real basis. In the natural supersymmetric basis, the λ_i of Eq. (A1) are given by

$$\begin{aligned}&\lambda_1 = \lambda_2 = \tfrac{1}{4}(g^2 + g'^2), \qquad \lambda_3 = \tfrac{1}{4}(g^2 - g'^2),\\ &\lambda_4 = -\tfrac{1}{2}g^2, \qquad \lambda_5 = \lambda_6 = \lambda_7 = 0,\end{aligned} \tag{D25}$$

where g and g' are the usual electroweak couplings [with $m_Z^2 = \frac{1}{4}(g^2 + g'^2)v^2$]. From these results, one can compute the (pseudo-)invariants:

$$\begin{aligned}&Z_1 = Z_2 = \tfrac{1}{4}(g^2 + g'^2)\cos^2 2\beta,\\ &Z_3 = Z_5 + \tfrac{1}{4}(g^2 - g'^2), \qquad Z_4 = Z_5 - \tfrac{1}{2}g^2,\\ &Z_5 = \tfrac{1}{4}(g^2 + g'^2)\sin^2 2\beta,\\ &Z_6 = -Z_7 = -\tfrac{1}{4}(g^2 + g'^2)\sin 2\beta\cos 2\beta.\end{aligned} \tag{D26}$$

The standard MSSM tree-level Higgs sector formulae [4] for the Higgs masses and $\beta - \alpha$ are easily reproduced using Eq. (D26) and the results of this appendix.

2. The decoupling limit of the 2HDM

The decoupling limit corresponds to the limiting case in which one of the two-Higgs doublets of the 2HDM receives a very large mass and is therefore decoupled from the theory [42,43]. This can be achieved by assuming that $Y_2 \gg v^2$ and $|Z_i| \lesssim \mathcal{O}(1)$ [for all i]. The effective low-energy theory is a one-Higgs-doublet model that corresponds to the Higgs sector of the standard model. We shall order the neutral scalar masses according to $m_1 < m_{2,3}$ and define the invariant Higgs mixing angles accordingly. Thus, we expect one light CP-even Higgs boson, h_1, with couplings identical (up to small corrections) to those of the standard model (SM) Higgs boson. Using the fact that m_1^2, $|Z_i|v^2 \ll m_2^2$, m_3^2, $m_{H^\pm}^2$ in the decoupling limit, Eqs. (C13) and (C14) yield[33]:

$$|s_{12}| \lesssim \mathcal{O}\left(\frac{v^2}{m_2^2}\right) \ll 1, \qquad |s_{13}| \lesssim \mathcal{O}\left(\frac{v^2}{m_3^2}\right) \ll 1, \tag{D27}$$

and Eq. (C23) implies that $\tan 2\phi + \tan 2\theta_{56} \ll 1$, where $\theta_{56} \equiv \frac{1}{2}\arg Z_5 - \arg Z_6$. This latter inequality is equivalent to

$$\mathrm{Im}\,(Z_5 e^{-2i\theta_{23}}) \lesssim \mathcal{O}\left(\frac{v^2}{m_3^2}\right) \ll 1. \tag{D28}$$

Note that Eq. (D28) is also satisfied if $\theta_{23} \to \theta_{23} + \pi/2$. These two respective solutions (modulo π) correspond to the two possible mass orderings of h_2 and h_3.

One can explicitly verify the assumed mass hierarchy of the Higgs bosons in the decoupling limit. Using Eqs. (C12) and (D27), it follows that $m_1^2 = Z_1 v^2$, with corrections $\lesssim \mathcal{O}(v^4/m_{2,3}^2)$. Equation (C26) yields $m_3^2 = A^2$, with corrections $\lesssim \mathcal{O}(v^2)$, and Eq. (C27) yields $m_3^2 - m_2^2 \lesssim \mathcal{O}(v^2)$. Finally, we employ Eqs. (23) and (42) to conclude that $m_{H^\pm}^2 - m_3^2 \lesssim \mathcal{O}(v^2)$. That is, $m_1 \ll m_2 \simeq m_3 \simeq m_{H^\pm}$.

The values of the $q_{k\ell}$ in the exact decoupling limit, where $s_{12} = s_{13} = \mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$, are tabulated in Table V. It is a simple exercise to insert the values of the $q_{k\ell}$ in the exact decoupling limit into the Higgs couplings of Secs. V and VI. The couplings of $h_1 \equiv h$ are then given by

$$\begin{aligned}\mathcal{L}_h =\, & \frac{1}{2}(\partial_\mu h)^2 - \frac{1}{2}Z_1 v^2 h^2 - \frac{1}{2}vZ_1 h^3 - \frac{1}{8}vZ_1 h^4\\ &+ \left(g m_W W_\mu^+ W^{\mu -} + \frac{g}{2c_W} m_Z Z_\mu Z^\mu\right)h\\ &+ \left[\frac{1}{4}g^2 W_\mu^+ W^{\mu -} + \frac{g^2}{8c_W^2} Z_\mu Z^\mu\right]h^2\\ &+ \left\{\left(\frac{1}{2}egA^\mu W_\mu^+ - \frac{g^2 s_W^2}{2c_W} Z^\mu W_\mu^+\right)G^- h + \mathrm{H.c.}\right\}\\ &- \frac{1}{2}ig[W_\mu^+ G^- \overleftrightarrow{\partial}^\mu h + \mathrm{H.c.}] + \frac{g}{2c_W} Z^\mu G^0 \overleftrightarrow{\partial}_\mu h\\ &+ \frac{1}{v}\bar{D}M_D D h + \frac{1}{v}\bar{U}M_U U h.\end{aligned} \tag{D29}$$

This is precisely the SM Higgs Lagrangian. Even in the most general CP-violating 2HDM, the interactions of the h in the decoupling limit are CP-conserving and diagonal in quark flavor space. CP-violating and flavor nondiagonal effects in the Higgs interactions are suppressed by factors of $\mathcal{O}(v^2/m_{2,3}^2)$ as shown in detail in Ref. [48]. In contrast to the SM-like Higgs boson h, the interactions of the heavy neutral Higgs bosons (h_2 and h_3) and the charged Higgs bosons ($H^\pm$) exhibit both CP-violating and quark flavor

[33] We assumed that $Z_6 \neq 0$ in the derivation of Eqs. (D27) and (D28). In the case of $Z_6 = 0$, we may use Eqs. (C21), (C25), and (D4) to conclude that $s_{12} = s_{13} = 0$ are exactly satisfied as long as $m_1 < m_{2,3}$. Setting Eq. (C6) to zero, it then follows that $\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$.

TABLE V. The U(2)-invariant quantities $q_{k\ell}$ in the exact decoupling limit.

k	q_{k1}	q_{k2}
1	1	0
2	0	1
3	0	i
4	i	0

nondiagonal couplings (proportional to the ρ^Q) in the decoupling limit. In particular, whereas Eq. (D28) implies that $\sin 2(\theta_5 - \theta_{23}) \ll 1$, the *CP*-violating invariant quantities $\sin(\theta_6 - \theta_{23})$ and $\sin(\theta_7 - \theta_{23})$ [c.f. Eq. (D2)] need not be small in the most general 2HDM.

One can understand the origin of the decoupling conditions [Eqs. (D27) and (D28)] as follows. First, using Eq. (C2), we see that we can decouple h_2 and h_3 (and $H^\pm$) by taking $A^2 \gg v^2$ while sending $q_{12} \to 0$. Thus, in the convention in which the mass ordering of the three neutral Higgs states is $m_1 \leq m_2 \leq m_3$, it follows that the exact decoupling limit is formally achieved when $A^2 \to \infty$ and $|q_{12}|^2 = s_{12}^2 + c_{12}^2 s_{13}^2 = 0$, which implies that $s_{12} = s_{13} = 0$. Inserting these results into Eq. (44) yields $\tilde{R} = I$, where I is the 3×3 identity matrix. Consequently, $\tilde{\mathcal{M}}$ [see Eqs. (41)–(43)] must be diagonal up to corrections of $\mathcal{O}(v^2/A^2)$. However, because Eq. (41) is dominated in the decoupling limit by its 22 and 33 elements (which are approximately degenerate), it follows that the 23 element must vanish exactly in leading order. Thus, in the exact decoupling limit, $\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$. Note that this latter constraint is consistent with Eq. (C8), as $\theta_{13} = 0$ in the decoupling limit.

For further details and a more comprehensive treatment of the decoupling limit, see Refs. [43,48].

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