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Basis-independent methods for the two-Higgs-doublet model III: The CP-conserving limit, custodial symmetry, and the oblique parameters S, T, U

Howard E. Haber and Deva O'Neil*

Santa Cruz Institute for Particle Physics
University of California, Santa Cruz, CA 95064, U.S.A.

In the Standard Model, custodial symmetry is violated by the hypercharge U(1) gauge interactions and the Yukawa couplings, while being preserved by the Higgs scalar potential. In the two-Higgs doublet model (2HDM), the generic scalar potential introduces new sources of custodial symmetry breaking. We obtain a basis-independent expression for the constraints that impose custodial symmetry on the 2HDM scalar potential. These constraints impose CP-conservation on the scalar potential and vacuum, and in addition add one extra constraint on the scalar potential parameters. We clarify the mass degeneracies of the 2HDM that arise as a consequence of the custodial symmetry. We also provide a computation of the "oblique" parameters (S, T, and U) for the most general CP-violating 2HDM in the basis-independent formalism. We demonstrate that the 2HDM contributions to T and U vanish in the custodial symmetry limit, as expected. Using the experimental bounds on S and T from precision electroweak data, we examine the resulting constraints on the general 2HDM parameter space.

1.   INTRODUCTION: THE CP-VIOLATING TWO HIGGS DOUBLET MODEL (2HDM)

In the most general two-Higgs-doublet extension of the Standard Model (2HDM), the two hypercharge-one Higgs doublet fields Φ_1 and Φ_2 are indistinguishable. Consequently, all physical observables must be independent of a change in the scalar basis, which corresponds to a redefinition of the scalar doublets by a global U(2) transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$. In refs. [1] and [2], a basis-independent formalism for the 2HDM was introduced and developed.[1] In particular, a basis-independent form for the most general 2HDM interactions was obtained in ref. [2]. A recap of the basis-independent formalism for the 2HDM is provided in Section 2 in order to make this paper self-contained.

However, the most general form of the 2HDM is certainly not realized in nature. For example, for generic 2HDM parameters, one expects large flavor-changing neutral currents and a significant violation of custodial symmetry, in conflict with experimental observations. These problems are ameliorated in restricted parameter regimes of the 2HDM. These restricted regions are either fine-tuned or can be implemented by imposing additional symmetries (e.g. discrete symmetries or supersymmetry) on the 2HDM scalar potential. Such additional symmetries would in general distinguish between the two-Higgs doublet fields, and thereby choose a preferred basis. If 2HDM phenomena are observed in nature, one important goal of experimental Higgs studies at future colliders will be to determine the nature of the additional symmetry structures (if present) that restrict the 2HDM parameters, and the associated preferred scalar basis. However, prior to determining whether such a preferred scalar basis exists, the basis-independent techniques will be critical for exploring the phenomenological profile of the 2HDM and determining its theoretical structure.

In this paper, we provide a basis-independent formulation of custodial symmetry for the most general 2HDM. If custodial symmetry were exact, then there would be no Higgs sector corrections to the tree-level relation $m_W^2 = m_Z^2 \cos^2 \theta_W$ to all orders in perturbation theory. Of course, custodial symmetry is not an exact symmetry of the Standard Model, as it is violated by the hypercharge gauge interactions and the Higgs–fermion Yukawa interactions. The precision measurements of electroweak observables by LEP and the Tevatron suggest that additional sources of custodial symmetry breaking beyond that which is contained in the Standard Model must be small. This imposes interesting constraints on the most general 2HDM.

The custodial symmetric 2HDM scalar potential must be CP-conserving. Thus, in Section 3 we first review the basis-independent conditions for a CP-conserving 2HDM potential. We then establish the basis-independent conditions for a custodial symmetric 2HDM scalar potential in Section 4. These results clarify the significance of the conditions for custodial symmetry in the 2HDM obtained previously in the literature [7]. The effects of the custodial symmetry-

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* Present address: Physics Department, Bridgewater College, Bridgewater, VA 22812.

[1] There is an alternative approach, which we do not employ in this paper, that emphasizes the role of gauge-invariant scalar field bilinears. For further details, see e.g. refs. [3–6].

violating terms on the 2HDM have phenomenological consequences. In particular, these terms would lead to shifts in the Peskin-Takeuchi T and U parameters [8]. In contrast, shifts in the S parameter [8] can be generated even in the presence of an exact custodial symmetry. In Section 5, we have obtained basis-independent expressions for the 2HDM contributions to the oblique parameters S, T and U. Using these results, we present in Section 6 a numerical study of the size of the 2HDM contributions to the oblique parameters as a function of the 2HDM parameter space. By comparing these results to the experimental bounds on S and T, we determine some of the features of the constraints on the 2HDM parameter space. Conclusions are given in Section 7.

Some details have been relegated to the appendices. In Appendix A, we reproduce the cubic and quartic bosonic couplings of the 2HDM obtained in ref. [2]. These couplings are critical for determining the CP-quantum numbers of the neutral Higgs states for the CP-conserving scalar potential. In Appendix B, we record some useful expressions involving the neutral Higgs masses and invariant mixing angles. In Appendix C we summarize the basis-independent treatment of the CP-conserving 2HDM. This appendix also examines a number of special cases in which some of the neutral Higgs scalars are mass-degenerate. Appendix D provides details of the computation of the 2HDM contributions to S, T and U, along with the relevant Feynman rules (in the basis-independent formalism) and one-loop graphs. Appendix E summarizes the key features of the decoupling limit of the 2HDM. Finally, in Appendix F, we examine the tree-level unitarity bounds on the scalar potential parameters in the basis-independent formalism. These bounds are implemented in the parameter space scans of Section 6.

2.   RECAP OF THE BASIS-INDEPENDENT FORMALISM FOR THE 2HDM

The scalar potential may be written in a basis-independent form as [1, 9]

$$\mathcal{V} = Y_{a\bar{b}}\Phi_{\bar{a}}^{\dagger}\Phi_b + \tfrac{1}{2}Z_{a\bar{b}c\bar{d}}(\Phi_{\bar{a}}^{\dagger}\Phi_b)(\Phi_{\bar{c}}^{\dagger}\Phi_d)\,, \tag{2.1}$$

where $Z_{a\bar{b}c\bar{d}} = Z_{c\bar{d}a\bar{b}}$ and hermiticity implies $Y_{a\bar{b}} = (Y_{b\bar{a}})^*$ and $Z_{a\bar{b}c\bar{d}} = (Z_{b\bar{a}d\bar{c}})^*$. The indices a, b, c and d label the two Higgs doublets, and there is an implicit sum over unbarred–barred index pairs. The barred indices help keep track of which indices transform with U and which transform with $U^{\dagger}$. For example, under a global U(2) transformation, the parameters of the scalar potential change according to

$$Y_{a\bar{b}} \rightarrow U_{a\bar{c}}Y_{c\bar{d}}U_{d\bar{b}}^{\dagger} \qquad \text{and} \qquad Z_{a\bar{b}c\bar{d}} \rightarrow U_{a\bar{e}}U_{f\bar{b}}^{\dagger}U_{c\bar{g}}U_{h\bar{d}}^{\dagger}Z_{e\bar{f}g\bar{h}}\,. \tag{2.2}$$

The vacuum expectation values of the two Higgs fields can be parametrized as

$$\langle\Phi_a\rangle = \frac{v}{\sqrt{2}}\begin{pmatrix} 0 \\ \widehat{v}_a \end{pmatrix}\,, \qquad \text{with} \qquad \widehat{v}_a \equiv e^{i\eta}\begin{pmatrix} \cos\beta \\ \sin\beta\, e^{i\xi} \end{pmatrix}\,, \tag{2.3}$$

where $v = 246$ GeV and η is an arbitrary phase. The unit vector $\widehat{v}_a$ satisfies $\widehat{v}_a\widehat{v}_{\bar{a}}^* = 1$, where $\widehat{v}_{\bar{a}}^* \equiv (\widehat{v}_a)^*$. If we define the hermitian matrix $V_{a\bar{b}} \equiv \hat{v}_a\hat{v}_{\bar{b}}^*$, then the scalar potential minimum condition is given by the invariant condition:

$$\text{Tr}(VY) + \tfrac{1}{2}v^2 Z_{a\bar{b}c\bar{d}}V_{b\bar{a}}V_{d\bar{c}} = 0\,. \tag{2.4}$$

The orthonormal eigenvectors of $V_{a\bar{b}}$ are $\hat{v}_b$ and

$$\widehat{w}_b \equiv \widehat{v}_{\bar{a}}^*\epsilon_{ab} = e^{-i\eta}\begin{pmatrix} -\sin\beta\, e^{-i\xi} \\ \cos\beta \end{pmatrix}\,, \tag{2.5}$$

where $\epsilon_{12} = -\epsilon_{21} = 1$ and $\epsilon_{11} = \epsilon_{22} = 0$. Under the U(2) transformation, $\widehat{v}_a \rightarrow U_{a\bar{b}}\hat{v}_b$, whereas

$$\widehat{w}_a \rightarrow (\det U)^{-1}\, U_{a\bar{b}}\,\widehat{w}_b\,,$$

where $\det U \equiv e^{i\chi}$ is a pure phase. That is, $\widehat{w}_a$ is a pseudo-vector with respect to global U(2) transformations. One can use $\widehat{w}_a$ and $\widehat{w}_{\bar{a}}^* \equiv (\widehat{w}_a)^*$ to construct a proper second-rank tensor, $W_{a\bar{b}} \equiv \widehat{w}_a\widehat{w}_{\bar{b}}^* \equiv \delta_{a\bar{b}} - V_{a\bar{b}}$.

One can always define the so-called Higgs basis in which only one of the two Higgs doublets has a neutral component with a non-zero vacuum expectation value [9, 10]. The Higgs basis fields are given by

$$H_1 = \widehat{v}_{\bar{a}}^*\Phi_a\,, \qquad\qquad H_2 = \widehat{w}_{\bar{a}}^*\Phi_a\,. \tag{2.6}$$

Since $\widehat{v}_a$ and $\widehat{w}_a$ are orthonormal vectors, it follows that

$$\langle H_1^0\rangle = \frac{v}{\sqrt{2}}\,, \qquad\qquad \langle H_2^0\rangle = 0\,. \tag{2.7}$$

Note that H_1 is an invariant field whereas $H_2 \to (\det U) H_2$ is a pseudo-invariant field under the global U(2) transformation. The scalar potential can then be expressed using the Higgs basis fields as follows:

$$\mathcal{V} = Y_1 H_1^\dagger H_1 + Y_2 H_2^\dagger H_2 + [Y_3 H_1^\dagger H_2 + \text{h.c.}]$$

$$+ \tfrac{1}{2} Z_1 (H_1^\dagger H_1)^2 + \tfrac{1}{2} Z_2 (H_2^\dagger H_2)^2 + Z_3 (H_1^\dagger H_1)(H_2^\dagger H_2) + Z_4 (H_1^\dagger H_2)(H_2^\dagger H_1)$$

$$+ \left\{ \tfrac{1}{2} Z_5 (H_1^\dagger H_2)^2 + \left[Z_6 (H_1^\dagger H_1) + Z_7 (H_2^\dagger H_2) \right] H_1^\dagger H_2 + \text{h.c.} \right\}, \tag{2.8}$$

where Y_1, Y_2 and $Z_{1,2,3,4}$ are real-valued U(2)-invariants,

$$Y_1 \equiv \text{Tr}(YV), \qquad\qquad Y_2 \equiv \text{Tr}(YW), \tag{2.9}$$

$$Z_1 \equiv Z_{a\bar{b}c\bar{d}} V_{b\bar{a}} V_{d\bar{c}}, \qquad\qquad Z_2 \equiv Z_{a\bar{b}c\bar{d}} W_{b\bar{a}} W_{d\bar{c}}, \tag{2.10}$$

$$Z_3 \equiv Z_{a\bar{b}c\bar{d}} V_{b\bar{a}} W_{d\bar{c}}, \qquad\qquad Z_4 \equiv Z_{a\bar{b}c\bar{d}} V_{b\bar{c}} W_{d\bar{a}} \tag{2.11}$$

and Y_3 and $Z_{5,6,7}$ are complex "pseudoinvariants,"

$$Y_3 \equiv Y_{a\bar{b}} \widehat{v}_a^* \widehat{w}_b, \qquad\qquad Z_5 \equiv Z_{a\bar{b}c\bar{d}} \widehat{v}_a^* \widehat{w}_b \widehat{v}_c^* \widehat{w}_d, \tag{2.12}$$

$$Z_6 \equiv Z_{a\bar{b}c\bar{d}} \widehat{v}_a^* \widehat{v}_b \widehat{v}_c^* \widehat{w}_d, \qquad\qquad Z_7 \equiv Z_{a\bar{b}c\bar{d}} \widehat{v}_a^* \widehat{w}_b \widehat{w}_c^* \widehat{w}_d. \tag{2.13}$$

which transform as

$$[Y_3, Z_6, Z_7] \to (\det U)^{-1} [Y_3, Z_6, Z_7] \qquad \text{and} \qquad Z_5 \to (\det U)^{-2} Z_5. \tag{2.14}$$

The scalar potential minimum condition [eq. (2.4)] fixes

$$Y_1 = -\tfrac{1}{2} Z_1 v^2, \qquad\qquad Y_3 = -\tfrac{1}{2} Z_6 v^2. \tag{2.15}$$

The three physical neutral Higgs boson mass-eigenstates can be determined by diagonalizing a 3×3 squared-mass matrix in the Higgs basis. The diagonalizing matrix is a 3×3 real orthogonal matrix that depends on three angles: θ_{12}, θ_{13} and θ_{23}. As shown in ref. [2], under a U(2) transformation,

$$\theta_{12}, \theta_{13} \text{ are invariant} \quad \text{and} \quad e^{i\theta_{23}} \to (\det U)^{-1} e^{i\theta_{23}}. \tag{2.16}$$

In particular, with respect to the *invariant* Higgs basis neutral fields $\{ \text{Re} \, \overline{H}_1^0, \text{Re}(e^{i\theta_{23}} H_2^0), \text{Im}(e^{i\theta_{23}} H_2^0) \}$, where $\overline{H}_1^0 \equiv H_1^0 - (v/\sqrt{2})$, the neutral Higgs squared-mass matrix is given by:

$$\mathcal{M}^2 = v^2 \begin{pmatrix} Z_1 & \text{Re}(Z_6 \, e^{-i\theta_{23}}) & -\text{Im}(Z_6 \, e^{-i\theta_{23}}) \\ \text{Re}(Z_6 e^{-i\theta_{23}}) & A^2/v^2 + \text{Re}(Z_5 \, e^{-2i\theta_{23}}) & -\tfrac{1}{2} \text{Im}(Z_5 \, e^{-2i\theta_{23}}) \\ -\text{Im}(Z_6 \, e^{-i\theta_{23}}) & -\tfrac{1}{2} \text{Im}(Z_5 \, e^{-2i\theta_{23}}) & A^2/v^2 \end{pmatrix}, \tag{2.17}$$

where

$$A^2 \equiv Y_2 + \tfrac{1}{2} [Z_3 + Z_4 - \text{Re}(Z_5 e^{-2i\theta_{23}})] v^2. \tag{2.18}$$

Note that $\mathcal{M}^2$ is manifestly basis-independent, in which case the neutral Higgs mass eigenstates are invariant fields with respect to U(2) transformations. Diagonalizing the neutral Higgs squared-mass matrix then gives

$$R \, \mathcal{M}^2 \, R^T = \mathcal{M}_D^2 = \text{diag}(m_1^2, m_2^2, m_3^2), \tag{2.19}$$

where m_1, m_2 and m_3 are the neutral Higgs boson masses and

$$R = \begin{pmatrix} c_{12} c_{13} & -s_{12} & -c_{12} s_{13} \\ s_{12} c_{13} & c_{12} & -s_{12} s_{13} \\ s_{13} & 0 & c_{13} \end{pmatrix}, \tag{2.20}$$

where $c_{ij} \equiv \cos \theta_{ij}$ and $s_{ij} \equiv \sin \theta_{ij}$. As shown in ref. [2], one can choose a convention (without loss of generality) where $-\tfrac{1}{2}\pi \le \theta_{12}, \theta_{13} < \tfrac{1}{2}\pi$. The neutral Goldstone boson is identified as $G^0 \equiv \text{Im} \, H_1^0$. One can express the mass eigenstate neutral Higgs bosons, h_k ($k = 1, 2, 3$) and the neutral Goldstone boson ($h_4 \equiv G^0$) directly in terms of the original shifted neutral fields, $\overline{\Phi}_a^0 \equiv \Phi_a^0 - v\widehat{v}_a/\sqrt{2}$,

$$h_k = \frac{1}{\sqrt{2}} \left[\overline{\Phi}_{\bar{a}}^{0\,\dagger} (q_{k1} \widehat{v}_a + q_{k2} \widehat{w}_a e^{-i\theta_{23}}) + (q_{k1}^* \widehat{v}_{\bar{a}}^* + q_{k2}^* \widehat{w}_{\bar{a}}^* e^{i\theta_{23}}) \overline{\Phi}_a^0 \right], \tag{2.21}$$

TABLE I: The U(2)-invariant quantities $q_{k\ell}$, defined in ref. [2], are reproduced below. The $q_{k\ell}$ are functions of the the invariant mixing angles θ_{12} and θ_{13}, where $c_{ij} \equiv \cos\theta_{ij}$ and $s_{ij} \equiv \sin\theta_{ij}$. By convention, we choose $-\frac{1}{2}\pi \leq \theta_{12}\,, \theta_{13} < \frac{1}{2}\pi$.

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

where $q_{k\ell}$ are basis-independent quantities composed of the invariant mixing angles θ_{12} and θ_{13} given in Table I.

The charged Goldstone and Higgs bosons are immediately identified in terms of Higgs basis fields as: $G^\pm \equiv H_1^\pm$ and $H^\pm = H_2^\pm$. The latter implies that $H^\pm \to (\det U)^{\pm 1} H^\pm$ under the U(2) transformation. If necessary, one can define an invariant charged Higgs field, $e^{\pm i\theta_{23}} H^\pm$. The charged Higgs mass is given by:

$$m_{H^\pm}^2 = Y_2 + \tfrac{1}{2}Z_3 v^2, \tag{2.22}$$

Finally, inverting eq. (2.21) yields:

$$\Phi_a = \begin{pmatrix} G^+ \widehat{v}_a + H^+ \widehat{w}_a \\[2mm] \dfrac{v}{\sqrt{2}}\widehat{v}_a + \dfrac{1}{\sqrt{2}}\sum_{k=1}^{4}\left(q_{k1}\widehat{v}_a + q_{k2}e^{-i\theta_{23}}\widehat{w}_a\right)h_k \end{pmatrix}. \tag{2.23}$$

Inserting this result into eq. (2.1) immediately yields the basis-independent form of the Higgs self-couplings given in Appendix A. Likewise, the invariant forms of the Higgs boson couplings to vector bosons can be obtained by expanding out the covariant derivatives that appear in the Higgs kinetic energy terms; these couplings are also given in Appendix A.

The Higgs boson couplings to the fermions arise from the Yukawa Lagrangian, which can be written in terms of the quark mass-eigenstate fields as:[2]

$$-\mathscr{L}_Y = \overline{U}_L \Phi_a^{0\,*} \eta_a^U U_R - \overline{D}_L K^\dagger \Phi_{\bar{a}}^- \eta_a^U U_R + \overline{U}_L K \Phi_a^+ \eta_{\bar{a}}^{D\,\dagger} D_R + \overline{D}_L \Phi_a^0 \eta_{\bar{a}}^{D\,\dagger} D_R + \text{h.c.}\,, \tag{2.24}$$

where K is the CKM mixing matrix. The $\eta^{U,D}$ are 3×3 Yukawa coupling matrices. We can construct invariant and pseudo-invariant matrix Yukawa couplings:

$$\kappa^Q \equiv \widehat{v}_{\bar{a}}^* \eta_a^Q\,, \qquad \rho^Q \equiv \widehat{w}_{\bar{a}}^* \eta_a^Q\,, \tag{2.25}$$

where $Q = U$ or D. Inverting these equations yields $\eta_a^Q = \kappa^Q \widehat{v}_a + \rho^Q \widehat{w}_a$. One can rewrite eq. (2.24) in the Higgs basis,[3]

$$-\mathscr{L}_Y = \overline{U}_L(\kappa^U H_1^{0\,\dagger} + \rho^U H_2^{0\,\dagger})U_R - \overline{D}_L K^\dagger(\kappa^U H_1^- + \rho^U H_2^-)U_R$$
$$+\overline{U}_L K(\kappa^{D\,\dagger} H_1^+ + \rho^{D\,\dagger} H_2^+)D_R + \overline{D}_L(\kappa^{D\,\dagger} H_1^0 + \rho^{D\,\dagger} H_2^0)D_R + \text{h.c.} \tag{2.26}$$

Note that under the U(2) transformation,

$$\kappa^Q \text{ is invariant and } \rho^Q \to (\det U)\rho^Q\,. \tag{2.27}$$

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,

$$M_U = \frac{v}{\sqrt{2}}\kappa^U = \text{diag}(m_u\,, m_c\,, m_t)\,, \qquad M_D = \frac{v}{\sqrt{2}}\kappa^{D\,\dagger} = \text{diag}(m_d\,, m_s\,, m_b)\,. \tag{2.28}$$

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[2] Eq. (2.24) corrects an error in eq. (75) of ref. [2].
[3] Eq. (2.26) corrects an error in eq. (76) of ref. [2].

The matrices ρ^U and ρ^D are independent complex 3×3 matrices. The final form for the Yukawa couplings of the mass-eigenstate Higgs bosons and the Goldstone bosons to the quarks is:

$$-\mathscr{L}_Y = \frac{1}{v}\overline{D}\left\{ M_D(q_{k1}P_R + q_{k1}^*P_L) + \frac{v}{\sqrt{2}}\left[q_{k2}\,[e^{i\theta_{23}}\rho^D]^\dagger P_R + q_{k2}^*\,e^{i\theta_{23}}\rho^D P_L\right]\right\}Dh_k$$

$$+\frac{1}{v}\overline{U}\left\{ M_U(q_{k1}P_L + q_{k1}^*P_R) + \frac{v}{\sqrt{2}}\left[q_{k2}^*\,e^{i\theta_{23}}\rho^U P_R + q_{k2}\,[e^{i\theta_{23}}\rho^U]^\dagger P_L\right]\right\}Uh_k$$

$$+\left\{ \overline{U}\left[K[\rho^D]^\dagger P_R - [\rho^U]^\dagger K P_L\right]DH^+ + \frac{\sqrt{2}}{v}\overline{U}\left[KM_D P_R - M_U K P_L\right]DG^+ + \text{h.c.}\right\}. \tag{2.29}$$

By writing $[\rho^Q]^\dagger H^+ = [\rho^Q e^{i\theta_{23}}]^\dagger [e^{i\theta_{23}}H^+]$, we see that the Higgs-fermion Yukawa couplings depend only on invariant quantities: the diagonal quark mass matrices, $\rho^Q e^{i\theta_{23}}$, and the invariant angles θ_{12} and θ_{13}. Since $\rho^Q e^{i\theta_{23}}$ is in general a complex matrix, eq. (2.29) contains CP-violating neutral-Higgs–fermion interactions. Moreover, eq. (2.29) exhibits Higgs-mediated flavor-changing neutral currents (FCNCs) at tree-level in cases where the ρ^Q are not flavor-diagonal. Thus, for a phenomenologically acceptable theory, the off-diagonal elements of ρ^Q must be small.

Note that the parameter $\tan\beta$ [where the angle β is defined in eq. (2.3)] does not appear in any of the Higgs couplings [cf. Appendix A and eq. (2.29)]. This is to be expected, since $\tan\beta$ is a basis-dependent quantity in the general 2HDM and is therefore an unphysical parameter [2]. Of course, $\tan\beta$ can be promoted to a physical parameter in special situations in which a particular basis is physical (e.g., in the presence of a discrete symmetry or supersymmetry, which restricts the form of the scalar potential in a particular basis). In this paper, we do not assume that any basis (apart from the Higgs basis and the neutral scalar mass-eigenstate basis) has physical significance.

3. BASIS-INDEPENDENT CONDITIONS FOR CP-CONSERVATION

At present, all known CP-violating effects can be attributed to a phase in the CKM matrix K. The source of this CP-violation is an unremovable complex phase in the Higgs–fermion Yukawa couplings of the Standard Model. When we extend the Standard Model by adding a second Higgs doublet, new sources of CP-violation can arise from potentially complex Higgs self-couplings and new Higgs–fermion Yukawa couplings. In this section, we determine the basis-independent conditions that yield no new sources of CP-violation (at tree-level) beyond the one non-trivial phase of the CKM matrix, and explore some of its consequences.

The Higgs scalar potential is explicitly CP-conserving if there exists a basis, called the *real basis*, in which all scalar potential parameters are simultaneously real [11]. In addition, if there exists a real basis in which the Higgs vacuum expectation values are simultaneously real, then CP is also preserved by the vacuum (and is not spontaneously broken). In the latter case, it is then possible to perform an O(2) global transformation on the fields of the Higgs basis, which maintains the reality of the scalar potential parameters. Hence, the condition for a CP-conserving Higgs potential and vacuum is the existence of a *real* Higgs basis. The only surviving basis freedom in defining the Higgs basis is the rephasing of H_2. Thus, it follows from eq. (2.8) that the Higgs scalar potential and vacuum are CP-conserving if and only if [4]

$$\text{Im}(Z_5^* Z_6^2) = \text{Im}(Z_5^* Z_7^2) = \text{Im}(Z_6^* Z_7) = 0\,, \tag{3.1}$$

which are equivalent to conditions first established in ref. [10], and subsequently rederived in refs. [1] and [11].

We now add in the Higgs-fermion interactions and impose the requirement of CP-conserving neutral Higgs boson-fermion interactions. This requirement is satisfied if the coefficients of the neutral Higgs boson-fermion interactions are simultaneously real in a real Higgs basis. It then follows from eq. (2.26) that [5]

$$Z_5(\rho^Q)^2\,,\ Z_6\,\rho^Q\,,\ \text{and}\ Z_7\,\rho^Q\ \text{are real matrices}\quad (Q = U, D\ \text{and}\ E)\,. \tag{3.2}$$

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[4] No separate condition is required for the complex parameter Y_3 due to the potential minimum condition of eq. (2.15).

[5] Eq. (3.2) corrects an error in eq. (D3) of ref. [2], which incorrectly stated that the matrices of eq. (3.2) must be hermitian. To derive this result, consider the interaction Lagrangian,

$$\mathscr{L}_{\text{int}} = A_{ij}\overline{Q}_i P_L Q_j + \text{h.c.},$$

and note that $(A_{ij}\overline{Q}_i P_L Q_j)^\dagger = A_{ij}^*\overline{Q}_j P_R Q_i = (A^\dagger)_{ij}\overline{Q}_i P_L Q_j$. Under a CP transformation,

$$U_{\text{CP}}(A_{ij}\overline{Q}_i P_L Q_j)U_{\text{CP}}^{-1} = A_{ij}\overline{Q}_j P_R Q_i = (A^T)_{ij}\overline{Q}_i P_R Q_j\,.$$

Imposing CP-invariance of the interaction Lagrangian yields $A^\dagger = A^T$; i.e., A is a real matrix.

Note that if eq. (3.2) is satisfied then $Z_5^{1/2}\rho^Q$ is either a purely real or a purely imaginary matrix. In particular, given a basis in which Z_5 is real and Z_6, Z_7 and the matrix ρ^Q are purely imaginary, one can always transform to a real Higgs basis via $H_2 \to iH_2$.

It is instructive to provide the explicit basis-independent form of the CP transformation law. In the Higgs basis, it is convenient to employ the invariant Higgs fields, H_1 and $e^{i\theta_{23}}H_2$. Then, under a CP transformation,

$$U_{\rm CP}H_1(\vec{\boldsymbol{x}},t)U_{\rm CP}^{-1} = H_1^\dagger(-\vec{\boldsymbol{x}},t)\,, \qquad U_{\rm CP}[\eta^* e^{i\theta_{23}}H_2(\vec{\boldsymbol{x}},t)]U_{\rm CP}^{-1} = [\eta^* e^{i\theta_{23}}H_2(-\vec{\boldsymbol{x}},t)]^\dagger\,, \qquad (3.3)$$

where $U_{\rm CP}$ is a unitary operator acting on the Hilbert space of fields, and η is a basis-independent complex phase factor to be determined. Applying this transformation to the Higgs scalar potential in the Higgs basis [eq. (2.8)], it follows that the Higgs scalar potential and vacuum is CP-invariant, i.e. $U_{\rm CP}\mathcal{V}U_{\rm CP}^{-1} = \mathcal{V}$ and $U_{\rm CP}|\,0\,\rangle = |\,0\,\rangle$, if

$$\mathrm{Im}(\eta^2 Z_5 e^{-2i\theta_{23}}) = 0\,, \qquad \mathrm{Im}(\eta Z_6 e^{-i\theta_{23}}) = 0\,, \qquad \mathrm{Im}(\eta Z_7 e^{-i\theta_{23}}) = 0\,. \qquad (3.4)$$

These results immediately yield the conditions of eq. (3.1). Likewise, if we demand that the neutral Higgs-fermion Yukawa interaction is CP-invariant, it follows that

$$\mathrm{Im}(\eta^* \rho^Q e^{i\theta_{23}}) = 0\,, \qquad (Q = U, D \text{ and } E)\,. \qquad (3.5)$$

Combining eqs. (3.4) and (3.5), we obtain the conditions of eq. (3.2).

In a generic basis, the CP transformation law is easily obtained by applying a global U(2) transformation to the Higgs basis fields in eq. (3.3). Using [2]

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} \widehat{w}_2 & -\widehat{w}_1 \\ -\widehat{v}_2 & \widehat{v}_1 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}. \qquad (3.6)$$

it follows that

$$\Phi_a(\vec{\boldsymbol{x}},t) \to (\widehat{v}_a\widehat{v}_b + \eta^2 e^{-2i\theta_{23}}\widehat{w}_a\widehat{w}_b)\Phi_{\bar{b}}^*(-\vec{\boldsymbol{x}},t)\,. \qquad (3.7)$$

One can easily check that the invariance of the scalar potential in the generic basis [eq. (2.1)] with respect to the transformation law of eq. (3.7) again yields eq. (3.1), as expected. Note that the matrix

$$\mathcal{U}_{ab} \equiv \widehat{v}_a\widehat{v}_b + \eta^2 e^{-2i\theta_{23}}\widehat{w}_a\widehat{w}_b\,, \qquad (3.8)$$

is unitary and symmetric. Thus, the CP-transformation law in the generic basis takes the general form (cf. ref. [11]):

$$U_{\rm CP}\Phi_a(\vec{\boldsymbol{x}},t)U_{\rm CP}^{-1} = \mathcal{U}_{ab}\Phi_{\bar{b}}^*(-\vec{\boldsymbol{x}},t)\,, \qquad (3.9)$$

and invariance of the vacuum under CP requires [9]:

$$\langle\Phi_a\rangle = \mathcal{U}_{ab}\langle\Phi_{\bar{b}}\rangle^*\,, \qquad (3.10)$$

where $\mathcal{U}$ is any symmetric unitary 2×2 matrix. Indeed, eq. (3.8) satisfies the above conditions.

If eqs. (3.1) and (3.2) are satisfied, then the neutral Higgs boson tree-level interactions are CP-conserving, and the neutral Higgs fields are eigenstates of CP. We follow the standard notation [12] and denote the CP-odd Higgs field by A^0 and the lighter and heavier CP-even neutral Higgs fields by h^0 and H^0, respectively.

The neutral Higgs mass eigenstates determine the mixing angles θ_{ij}. Thus, in the CP-conserving case, the requirement[6] that the neutral Higgs bosons are CP-eigenstates determines the phase factor η that appears in eqs. (3.3), (3.4), (3.7), (3.8) and (3.11). By examining the Higgs interaction terms given in Appendix A, one can determine a consistent set of assignments for the CP quantum numbers of the neutral Higgs bosons such that their interactions with gauge bosons and Higgs bosons is CP-invariant. For example, the CP-odd Higgs boson can be identified in general as[7]

$$A^0 = \mathrm{Im}(\eta^* e^{i\theta_{23}}H_2^0)\,. \qquad (3.11)$$

In Sections 3.1–3.3, we have examined all possible cases for the Higgs scalar parameters in which the scalar potential and vacuum is CP-conserving, and for each case the value of the phase factor η^2 is determined. For simplicity, we assume that the three neutral Higgs masses are non-degenerate. The mass-degenerate cases are treated in Appendix C.

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[6] In the case of non-degenerate neutral Higgs boson masses, it is automatic that the neutral Higgs mass eigenstates are simultaneously CP-eigenstates. In the case where the CP-odd Higgs boson is mass-degenerate with a CP-even Higgs boson, it is always convenient (though not strictly necessary) to choose the physical mass-degenerate states to be CP-eigenstates.

[7] In the case of $Z_6 = Z_7 = \rho^Q = 0$, one of the three neutral Higgs bosons is CP-even and the the other two neutral Higgs bosons have opposite CP quantum numbers. But for this special case, one cannot determine which of these latter two scalars is CP-odd. See Section 3.2 for further details.

3.1. The CP-conserving 2HDM with $Z_6 \neq 0$

For $Z_6 \neq 0$ (and no restrictions on the possible values of Z_5 or Z_7), a CP-invariant Higgs potential can arise in the 2HDM under one of the three cases listed in Table II. The derivation of these results (given in ref. [2]) is reviewed in Appendix C. Note that eqs. (3.4) and (3.5) correlate the overall phases of Z_6, Z_7 and the ρ^Q. In particular, in Case I, $\text{Im}(Z_6 e^{-i\theta_{23}}) = \text{Im}(Z_7 e^{-i\theta_{23}}) = \text{Im}(\rho^Q e^{i\theta_{23}}) = 0$, whereas $\text{Re}(Z_6 e^{-i\theta_{23}}) = \text{Re}(Z_7 e^{-i\theta_{23}}) = \text{Re}(\rho^Q e^{i\theta_{23}}) = 0$ in Cases IIa and b.

The U(2)-invariant quantities $q_{k\ell}$ for each of the three cases shown in Table II are exhibited in Tables III, IV and V.

TABLE II: Basis-independent conditions for a CP-conserving scalar potential and vacuum when $Z_6 \neq 0$. The neutral Higgs mixing angles θ_{ij} are defined with respect to the mass-ordering $m_{h_1} \leq m_{h_2} \leq m_{h_3}$. The phase factor η^2 governs the CP transformation law [cf. eq. (3.7)]. Additional conditions in which Z_6 is replaced by Z_7 and by ρ^{Q*} ($Q = U, D$ or E), respectively, must also hold due to the phase correlations implicit in eqs. (3.4) and (3.5). In the case where two of the neutral Higgs masses are equal, one linear combination of neutral Higgs states will be CP-even and the orthogonal linear combination will be CP-odd. The latter defines the relevant mixing angle, θ_{12} in Case I and θ_{13} in Case II, respectively.

Cases	conditions	η^2	A^0	h^0	H^0
I	$s_{13} = \text{Im}(Z_5\,e^{-2i\theta_{23}}) = \text{Im}(Z_6\,e^{-i\theta_{23}}) = 0$	$+1$	h_3	h_1	h_2
IIa	$s_{12} = \text{Im}(Z_5\,e^{-2i\theta_{23}}) = \text{Re}(Z_6\,e^{-i\theta_{23}}) = 0$	-1	h_2	h_1	h_3
IIb	$c_{12} = \text{Im}(Z_5\,e^{-2i\theta_{23}}) = \text{Re}(Z_6\,e^{-i\theta_{23}}) = 0$	-1	h_1	h_2	h_3

TABLE III: The U(2)-invariant quantities $q_{k\ell}$ for Case I

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

TABLE IV: The U(2)-invariant quantities $q_{k\ell}$ for Case IIa

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

TABLE V: The U(2)-invariant quantities $q_{k\ell}$ for Case IIb

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

It is convenient to define an invariant quantity, ε_{56}, by the relation

$$\text{Re}(Z_5^* Z_6^2) = \varepsilon_{56}|Z_5|\,|Z_6|^2\,, \qquad \varepsilon_{56} \equiv \pm 1\,. \tag{3.12}$$

Since $\text{Im}\,(Z_5 e^{-2i\theta_{23}}) = 0$ is satisfied in Cases I and II, it follows that

$$\text{Re}(Z_5^* Z_6^2) = \text{Re}(Z_5 e^{-2i\theta_{23}})\left[\text{Re}(Z_6 e^{-i\theta_{23}})^2 - \text{Im}(Z_6 e^{-i\theta_{23}})^2\right] = \pm|Z_6|^2 \text{Re}(Z_5 e^{-2i\theta_{23}})\,, \tag{3.13}$$

where we take the positive [negative] sign depending on whether $\text{Im}(Z_6\,e^{-i\theta_{23}}) = 0$ [$\text{Re}(Z_6\,e^{-i\theta_{23}}) = 0$]. Hence, eqs. (3.12) and (3.13) yield

$$\text{Re}(Z_5 e^{-2i\theta_{23}}) = \begin{cases} \epsilon_{56}|Z_5|\,, & \text{if } \text{Im}(Z_6\,e^{-i\theta_{23}}) = 0\,, \\ -\epsilon_{56}|Z_5|\,, & \text{if } \text{Re}(Z_6\,e^{-i\theta_{23}}) = 0\,. \end{cases} \tag{3.14}$$

Note that ε_{56} is the sign of Z_5 in the real basis.[8] Eq. (3.14) can be rewritten more compactly as:

$$\text{Re}(Z_5 e^{-2i\theta_{23}}) = \eta^2 \epsilon_{56}|Z_5|\,. \tag{3.15}$$

One can use eq. (3.11) to identify the CP-odd Higgs boson, A^0. The identity of A^0 is also easily discerned from Tables III, IV and V, since any neutral Higgs state h_k with $q_{k1} \neq 0$ must be CP-even. As there is one CP-odd state in the neutral Higgs spectrum, it must correspond to the $q_{k1} = 0$ entries of Tables III, IV and V.

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[8] In the real Higgs basis as defined above, $\theta_{23} = n\pi$ for integer n. Since $\text{Im}(Z_5 e^{-2i\theta_{23}}) = 0$, it follows from eq. (3.14) that $Z_5 = \epsilon_{56}|Z_5|$. That is, ε_{56} is the sign of Z_5 in the real Higgs basis.

The squared-masses of the neutral bosons are given by:

$$m^2_{h^0, H^0} = \tfrac{1}{2}v^2 \left[Y_2/v^2 + Z_1 + \tfrac{1}{2}(Z_3 + Z_4 + \varepsilon_{56}|Z_5|) \mp \sqrt{\left[Y_2/v^2 - Z_1 + \tfrac{1}{2}(Z_3 + Z_4 + \varepsilon_{56}|Z_5|) \right]^2 + 4|Z_6|^2} \right],$$
(3.16)

$$m^2_{A^0} = Y_2 + \tfrac{1}{2}v^2(Z_3 + Z_4 - \varepsilon_{56}|Z_5|),$$
(3.17)

where ϵ_{56} is defined above [cf. eqs. (3.12) and (3.14)]. In particular, Case I corresponds to the mass ordering $m_{A^0} > m_{H^0}$, and Cases IIa and IIb correspond to $m_{A^0} < m_{H^0}$. Moreover, the two separate parameter regimes corresponding to Cases IIa and IIb correspond to the two possible mass orderings $m_{A^0} < m_{h^0}$ and $m_{A^0} > m_{h^0}$, respectively, as exhibited in Table II.

3.2. The CP-conserving 2HDM with $Z_6 = 0$ and $Z_7 \neq 0$

For the case of $Z_6 = 0$ and $Z_7 \neq 0$, a CP-invariant Higgs potential can arise in the 2HDM under any one of the following six conditions listed in Table VI. The U(2)-invariant quantities $q_{k\ell}$ for the cases shown in Table VI are exhibited in Tables VII, VIII and IX. A derivation of these results is given in Appendix C.

TABLE VI: Basis-independent conditions for a CP-conserving scalar potential and vacuum when $Z_6 = 0$, $Z_7 \neq 0$. The neutral Higgs mixing angles θ_{ij} are defined with respect to the mass-ordering $m_{h_1} \leq m_{h_2} \leq m_{h_3}$, and $\overline{\theta}_{23} \equiv \theta_{23} - \theta_{12}$. The phase factor η^2 governs the CP transformation law [cf. eq. (3.7)]. Additional conditions in which Z_7 is replaced by ρ^{Q*} ($Q = U, D$ and E), respectively, must also hold due to the phase correlations implicit in eqs. (3.19) and (3.20). The two CP-even states are denoted as h_1^0 and h_2^0, where $m^2_{h_1^0} = Z_1 v^2$ and $m^2_{h_2^0} = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 + \varepsilon_{57}|Z_5|)v^2$. The couplings of h_1^0 coincide with those of the Standard Model Higgs boson. The squared-mass of the CP-odd Higgs boson is given by: $m^2_{A^0} = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 - \varepsilon_{57}|Z_5|)v^2$. If Z_1 is chosen such that h_1^0 is degenerate in mass with either h_2^0 or A^0, then θ_{12} in Cases I' and II' or θ_{13} in Case III' are fixed by the requirement that the properties of the mass-degenerate state h_1^0 coincide with those of the Standard Model Higgs boson. Additional cases not included in this table that can arise when two of the neutral Higgs bosons are degenerate in mass are treated in Table XIII.

Cases	conditions	η^2	A^0	h_1^0	h_2^0
I'a	$s_{13} = s_{12} = \mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = \mathrm{Im}(Z_7\, e^{-i\theta_{23}}) = 0$	$+1$	h_3	h_1	h_2
I'b	$s_{13} = s_{12} = \mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = \mathrm{Re}(Z_7\, e^{-i\theta_{23}}) = 0$	-1	h_2	h_1	h_3
II'a	$s_{13} = c_{12} = \mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = \mathrm{Im}(Z_7\, e^{-i\theta_{23}}) = 0$	$+1$	h_3	h_2	h_1
II'b	$s_{13} = c_{12} = \mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = \mathrm{Re}(Z_7\, e^{-i\theta_{23}}) = 0$	-1	h_1	h_2	h_3
III'a	$c_{13} = \mathrm{Im}(Z_5\, e^{-2i\overline{\theta}_{23}}) = \mathrm{Im}(Z_7\, e^{-i\overline{\theta}_{23}}) = 0$	$e^{2i\theta_{12}}$	h_1	h_3	h_2
III'b	$c_{13} = \mathrm{Im}(Z_5\, e^{-2i\overline{\theta}_{23}}) = \mathrm{Re}(Z_7\, e^{-i\overline{\theta}_{23}}) = 0$	$-e^{2i\theta_{12}}$	h_2	h_3	h_1

TABLE VII: The U(2)-invariant quantities $q_{k\ell}$ for Cases I'a and I'b

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

TABLE VIII: The U(2)-invariant quantities $q_{k\ell}$ for Cases II'a and II'b

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

TABLE IX: The U(2)-invariant quantities $q_{k\ell}$ for Cases III'a and III'b

k	q_{k1}	q_{k2}
1	0	$ie^{i\theta_{12}}$
2	0	$e^{i\theta_{12}}$
3	-1	0

Cases I′a and I′b correspond to the combination of Cases I and IIa of Table II. Cases II′a and II′b correspond to the combination of Cases I and IIb of Table II. Finally, Cases III′a and III′b are new. In these last two cases,

$$\overline{\theta}_{23} \equiv \theta_{23} - \theta_{12}\,, \qquad \overline{\eta}^2 = \eta^2 e^{-2i\theta_{12}} = \pm 1\,, \tag{3.18}$$

play the roles of θ_{23} and η^2, respectively. Note that eqs. (3.4) and (3.5) correlate the overall phases of Z_7 and the ρ^Q. In particular,

Cases I′a and II′a: $\text{Im}(Z_7 e^{-i\theta_{23}}) = \text{Im}(\rho^Q e^{i\theta_{23}}) = 0$, Case III′a: $\text{Im}(Z_7 e^{-i\overline{\theta}_{23}}) = \text{Im}(\rho^Q e^{i\overline{\theta}_{23}}) = 0$, (3.19)

Cases I′b and II′b: $\text{Re}(Z_7 e^{-i\theta_{23}}) = \text{Re}(\rho^Q e^{i\theta_{23}}) = 0$, Case III′b: $\text{Re}(Z_7 e^{-i\overline{\theta}_{23}}) = \text{Re}(\rho^Q e^{i\overline{\theta}_{23}}) = 0$. (3.20)

The Higgs state corresponding to $q_{k1} \neq 0$ in Tables VII, VIII and IX is a CP-even Higgs boson. Moreover, as $q_{k1} = \pm 1$ and $|q_{k2}| = 0$ in each case, it follows from Appendix A that this state has precisely the couplings of the Standard Model Higgs boson! Note that the q_{k1} vanish for the other two neutral Higgs states, and thus cannot be used to fix the absolute CP quantum numbers of these two states. In the $Z_6 = 0$ model, it is Z_7 and/or ρ^Q that determine which of these two states is CP-even and which is CP-odd.

It is convenient to define an invariant quantity, ε_{57}, by the relation

$$\text{Re}(Z_5^* Z_7^2) = \varepsilon_{57}|Z_5|\,|Z_7|^2\,, \qquad \varepsilon_{57} \equiv \pm 1\,. \tag{3.21}$$

Since $\text{Im}(Z_5 e^{-2i\theta_{23}}) = 0$ is satisfied in Cases I′ and II′, it follows that

$$\text{Re}(Z_5 e^{-2i\theta_{23}}) = \begin{cases} \epsilon_{57}|Z_5|\,, & \text{if } \text{Im}(Z_7 e^{-i\theta_{23}}) = 0\,, \\ -\epsilon_{57}|Z_5|\,, & \text{if } \text{Re}(Z_7 e^{-i\theta_{23}}) = 0\,. \end{cases} \tag{3.22}$$

Note that ε_{57} is the sign of Z_5 in the real basis. Eq. (3.22) can be rewritten more compactly as:

$$\text{Re}(Z_5 e^{-2i\theta_{23}}) = \eta^2 \epsilon_{57}|Z_5|\,. \tag{3.23}$$

In Case III′, $\text{Im}(Z_5 e^{-2i\overline{\theta}_{23}}) = 0$, in which case, eqs. (3.22) and (3.23) hold with θ_{23} and η^2 are replaced by $\overline{\theta}_{23}$ and $\overline{\eta}^2$, respectively.

The masses of the neutral Higgs bosons are as follows. There is one CP-even Higgs boson whose squared-mass is given by:[9]

$$m_{h_1^0}^2 = Z_1 v^2\,. \tag{3.24}$$

As noted above, the mass and couplings of h_1^0 are exactly the same as those of the Standard Model Higgs boson.[10] The squared-masses of the remaining two neutral Higgs bosons (a CP-even state h_2^0 and a CP-odd state A^0) are given by:

$$m_{h_2^0}^2 = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 + \varepsilon_{57}|Z_5|)v^2\,, \tag{3.25}$$

$$m_{A^0}^2 = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 - \varepsilon_{57}|Z_5|)v^2\,. \tag{3.26}$$

Cases involving mass-degenerate neutral Higgs bosons are examined in Appendix C.

The above results are valid as long as either Z_6 or Z_7 is non-vanishing. If both $Z_6 = 0$ and $Z_7 = 0$, the model has some extra features, which we examine in the following section.

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[9] In eqs. (3.24) and (3.25), we employ the notation h_1^0 and h_2^0 for the two CP-even Higgs bosons (rather than h^0 and H^0), since the mass ordering of these states depends on the the choice of the 2HDM parameters.

[10] The Standard Model properties of h_1^0 are independent of its mass and the masses of h_2^0 and A^0. In this sense, this case is not a decoupling limit, although the properties of h_1^0 are identical to the corresponding properties of the lightest CP-even Higgs boson in the decoupling limit.

3.3. The 2HDM with $Z_6 = Z_7 = 0$

In Sections 3.1 and 3.2, we established basis-independent conditions for which the 2HDM scalar potential and vacuum were CP-conserving. If $Z_6 = Z_7 = 0$ (and $Y_3 = 0$ by virtue of the potential minimum condition), then Z_5 is the the only potentially complex parameter of the scalar potential in the Higgs basis. Consequently, one can rephase the Higgs field H_2 to obtain a real Higgs basis (where Z_5 is real). Hence, if $Z_6 = Z_7 = 0$ then the 2HDM scalar potential and vacuum automatically preserve the CP symmetry.[11]

Starting from any real basis of a CP-invariant 2HDM scalar potential, one can always apply an O(2) transformation to the Higgs fields to define another generic real basis. In general, all possible real basis choices can be reached in this way. However, in the case of $Y_3 = Z_6 = Z_7 = 0$, there exists a particular U(2) transformation, $\mathrm{diag}(1, i)$, that is not an O(2) transformation, which has the effect of changing the sign of Z_5. This corresponds to redefining the second Higgs field by

$$H_2 \to iH_2. \tag{3.27}$$

Following Appendix A of ref. [11] (where the analogous arguments for the time-reversal-invariant 2HDM is presented), the CP transformation law is unique only if all real basis choices are related by an O(2) transformation. If all real basis choices are related by a larger global transformation group, $\mathrm{O}(2) \times \mathbb{D} \subset \mathrm{U}(2)$, then the CP transformation law (within the Higgs/gauge boson sector) is not unique and the number of inequivalent CP transformation laws is equal to the number of elements of the (non-trivial) discrete group $\mathbb{D}$. Applying this to the 2HDM with $Y_3 = Z_6 = Z_7 = 0$, we identify $\mathbb{D} = \mathbb{Z}_2$, which is the discrete group consisting of the identity element and $\mathrm{diag}(1, i) \in \mathrm{U}(2)$ [the latter changes the sign of Z_5]. We conclude that for the $Y_3 = Z_6 = Z_7 = 0$ model, there are two inequivalent definitions of CP in the Higgs/gauge boson sector. For example, in Cases I' and II' of Table VI, the two definitions of CP correspond to $\eta^2 = \pm 1$ in eq. (3.7) [for Case III', simply replace θ_{23} with $\overline{\theta}_{23}$ and η^2 with $\overline{\eta}^2$].

In particular, consider the U(2)-invariant couplings $q_{k\ell}$ given in Tables VII, VIII and IX. The Higgs boson h_1^0, defined here as the scalar h_k corresponding to $|q_{k1}| = 1$, is CP-even. For either choice of the two inequivalent definitions of CP, the couplings of h_1^0 precisely match those of the Standard Model Higgs boson [as previously noted below eq. (3.20)]. But, for the two Higgs states h_2^0 and h_3^0 with $q_{k1} = 0$, the Higgs/gauge boson interactions are insufficient to uniquely identify the CP-odd Higgs field as noted above. The squared-mass of the neutral Higgs bosons must be the same as in the previous subsection (where $Z_6 = 0$ and $Z_7 \neq 0$), since the neutral Higgs squared-mass matrix is independent of Z_7. However, when $Z_7 = 0$, we cannot employ eqs. (3.25) and (3.26) since ε_{57} is no longer defined. Nevertheless, one can directly analyze the squared-mass matrix given by eq. (2.17), which is diagonal. Defining $Z_5 \equiv |Z_5|e^{2i\theta_5}$, and noting that $\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$, it follows that $\theta_5 - \theta_{23} = \frac{1}{2}n\pi$ for some integer n. Hence $\mathrm{Re}(Z_5 e^{-2i\theta_{23}}) = \pm|Z_5|$, where the $\pm$ corresponds to the two possible choices $\theta_5 - \theta_{23} = 0$ or $\frac{1}{2}\pi$. We conclude that the squared-masses of h_2^0 and h_3^0 are given by:

$$m_{h_2^0, h_3^0}^2 = Y_2 + \tfrac{1}{2}v^2(Z_3 + Z_4 \mp |Z_5|), \tag{3.28}$$

where by convention, we choose $m_{h_2^0} < m_{h_3^0}$.

If the neutral Higgs–fermion Yukawa interactions are CP-conserving, then the ambiguity of the CP quantum numbers of h_2^0 and h_3^0 can be resolved. The results of Table VI still apply if Z_7 is replaced by ρ^{Q*} (for either $Q = U, D$ or E). It is convenient to define an invariant quantity, ε_{5Q}, by the relation,

$$\mathrm{Re}[Z_5 (\rho_{ij}^Q)^2] = \varepsilon_{5Q}|Z_5| \, |\rho_{ij}^Q|^2, \qquad \varepsilon_{5Q} \equiv \pm 1, \tag{3.29}$$

where ρ_{ij}^Q is any non-vanishing matrix element of ρ^Q. Following the derivation of eqs. (3.21), (3.22) and (3.23), it then follows that

$$\mathrm{Re}(Z_5 e^{-2i\theta_{23}}) = \begin{cases} \epsilon_{5Q}|Z_5|, & \text{if } \mathrm{Im}(e^{i\theta_{23}}\rho^Q) = 0, \\ -\epsilon_{5Q}|Z_5|, & \text{if } \mathrm{Re}(e^{i\theta_{23}}\rho^Q) = 0, \end{cases} \tag{3.30}$$

for Cases I' and II' (for Case III', θ_{23} and η^2 are replaced by $\overline{\theta}_{23}$ and $\overline{\eta}^2$, respectively). Note that ε_{5Q} is the sign of Z_5 in the real Higgs basis in which the scalar potential parameters and the Higgs-fermion Yukawa coupling matrices

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[11] One can implement $Y_3 = Z_6 = Z_7 = 0$ by imposing a $\mathbb{Z}_2$ symmetry in the Higgs basis. If the Higgs-fermion couplings also respect this discrete symmetry, then the resulting 2HDM is the Inert Doublet Model [13], since the model contains no interaction vertices with an odd number of H_2 fields.

are simultaneously real. In particular, ε_{5Q} is independent of the choice of i and j in eq. (3.29) [assuming $\rho_{ij}^Q \neq 0$]. Even though $Z_6 = Z_7 = 0$, the sign of Z_5 in the real Higgs basis is meaningful due to the presence of the Yukawa couplings. Eq. (3.30) can be rewritten more compactly as:

$$\mathrm{Re}(Z_5 e^{-2i\theta_{23}}) = \eta^2 \epsilon_{5Q} |Z_5|. \tag{3.31}$$

The two choices of $\eta^2 = \pm 1$ are now distinguishable. For example, in Case I′, the diagonal parts of the QQh_k interactions are given by:

$$\mathcal{L}_{QQh_2} = \frac{-1}{\sqrt{2}} \sum_{i=1}^{3} \overline{Q}_i \left[\mathrm{Re}(e^{i\theta_{23}} \rho^Q) \pm i\gamma_5 \mathrm{Im}(e^{i\theta_{23}} \rho^Q) \right]_{ii} Q_i h_2, \tag{3.32}$$

$$\mathcal{L}_{QQh_3} = \frac{-1}{\sqrt{2}} \sum_{i=1}^{3} \overline{Q}_i \left[\mp i\gamma_5 \mathrm{Re}(e^{i\theta_{23}} \rho^Q) + \mathrm{Im}(e^{i\theta_{23}} \rho^Q) \right]_{ii} Q_i h_3, \tag{3.33}$$

where the upper (lower) sign corresponds to $Q = U$ ($Q = D, E$). It follows that in Case I′, h_3 is CP-odd if $\eta^2 = 1$, i.e. $\mathrm{Im}(e^{i\theta_{23}} \rho^Q) = 0$ and h_2 is CP-even if $\eta^2 = -1$, i.e. $\mathrm{Re}(e^{i\theta_{23}} \rho^Q) = 0$. That is, the neutral-Higgs-fermion Yukawa interaction selects one of the two inequivalent definitions of CP. Cases II′ and III′ can be similarly treated. In a real Higgs basis, the unique CP transformation law depends on whether ρ^Q is a purely real or purely imaginary matrix. If the neutral Higgs–fermion Yukawa interactions are CP-violating, then neither h_2^0 nor h_3^0 can be assigned a definite CP quantum number.

3.4. CP symmetries in the 2HDM

Generalized CP-transformations (GCPs) in the 2HDM have been examined in refs. [14] and [15]. In a generic basis, a GCP transformation is of the form given in eq. (3.9), where $\mathcal{U}$ is an arbitrary 2×2 unitary matrix. Three classes of GCPs were identified in refs. [14] and [15] according to the value of $\mathcal{U}\mathcal{U}^*$:

$$\text{(i)} \quad \text{CP1}: \quad \mathcal{U}\mathcal{U}^* = \mathbb{1}_{2\times 2}, \quad \text{i.e., } \mathcal{U} \text{ is a unitary symmetric matrix}, \tag{3.34}$$

$$\text{(ii)} \quad \text{CP2}: \quad \mathcal{U}\mathcal{U}^* = -\mathbb{1}_{2\times 2}, \quad \text{i.e., } \mathcal{U} \text{ is a unitary antisymmetric matrix}, \tag{3.35}$$

$$\text{(iii)} \quad \text{CP3}: \quad \mathcal{U}\mathcal{U}^* \neq \pm\mathbb{1}_{2\times 2}, \tag{3.36}$$

where $\mathbb{1}_{2\times 2}$ is the 2×2 identity matrix. The CP1 transformation corresponds to eq. (3.8). Imposing CP1 on the 2HDM scalar potential implies that there exists a basis in which all the scalar potential parameters are real. Imposing CP2 and CP3 yields additional constraints on the scalar potential, which are not especially relevant to the matters addressed in this paper. In ref. [15], the possibility of imposing symmetries in a specific basis is discussed. This can lead to additional conditions on the scalar potential parameters, which may or may not correspond to a higher symmetry of the 2HDM.

In refs. [16] and [17], the CP1 transformation is applied directly in the Higgs basis. In particular, these authors examine:

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} e^{i\xi} & 0 \\ 0 & e^{-i\xi} \end{pmatrix} \begin{pmatrix} H_1^* \\ H_2^* \end{pmatrix}, \tag{3.37}$$

where $0 \leq \xi \leq \pi$. Imposing this CP1 transformation on the Higgs basis constrains the potentially complex scalar potential parameters as follows:

1. If $\xi = 0 \quad \implies \quad Y_3, Z_5, Z_6, Z_7 \in \mathbb{R},$ \hfill (3.38)

2. If $\xi = \pi \quad \implies \quad Z_5 \in \mathbb{R}, \quad Y_3 = Z_6 = Z_7 = 0,$ \hfill (3.39)

3. If $\xi \neq 0, \pi \quad \implies \quad Y_3 = Z_5 = Z_6 = Z_7 = 0.$ \hfill (3.40)

This analysis singles out the importance of the $Z_6 = Z_7 = 0$ model discussed in Section 3.3, which is designated as a "twisted" CP-conserving model in ref. [16].[12] The case of $Z_5 = Z_6 = Z_7 = 0$ possesses similar properties to the former model, with the added feature that the two Higgs scalars of indefinite CP quantum number are mass-degenerate.

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[12] In ref. [16], the twisted model is associated with the $Z_6 = Z_7 = 0$ model with custodial symmetry. Here, we see that custodial symmetry has nothing to do with the existence of this class of models, but is an additional constraint that can be imposed on the CP-conserving scalar potential. See Section 4.1.3 for further discussions of this point.

4. BASIS-INDEPENDENT CONDITIONS FOR CUSTODIAL SYMMETRY IN THE 2HDM

In the Standard Model, the tree-level relation, $m_W^2 = m_Z^2 \cos\theta_W$, is a consequence of an accidental global symmetry of the Higgs potential. In particular, the SM Higgs Lagrangian possesses an SO(4)$\cong$SU(2)$_L \times$SU(2)$_R/\mathbb{Z}_2$ global symmetry, whereas the full electroweak Lagrangian is invariant under SU(2)$\times$U(1)$_Y$, which is a subgroup of the larger global symmetry group. The global *custodial* SU(2)$_V$ symmetry, which is the diagonal (vector) subgroup of SU(2)$_L \times$SU(2)$_R$ (where $V = L + R$), is responsible for the gauge boson tree-level mass relation.

The U(1)$_Y$ hypercharge gauge interactions and the Higgs–fermion Yukawa couplings break the custodial symmetry. This leads to finite one-loop radiative corrections to the gauge boson tree-level mass relation. The dominant part of these corrections can be parameterized by a single quantity called T, introduced by Peskin and Takeuchi [8]. It is convenient to define T relative to a "reference Standard Model," in which the Higgs mass is fixed. A convenient choice is to define $T = 0$ for a Standard Model Higgs mass of 117 GeV.[13] Deviations from $T = 0$ can be accommodated by either changing the value of the Higgs mass or adding new custodial-violating interactions to the theory. Experimentally, T is observed to be quite small, which suggests that the custodial-breaking effects of the electroweak Lagrangian due to new physics beyond the Standard Model (or a Standard Model Higgs mass that differs significantly from 117 GeV) must be quite small.

In the 2HDM with a generic scalar potential, the Higgs Lagrangian does not possess a global custodial symmetry. One can therefore write the Higgs Lagrangian in the form

$$\mathcal{L}_{\text{Higgs}} = \mathcal{L}_{\text{CSC}} + \mathcal{L}_{\text{CSV}} , \tag{4.1}$$

where $\mathcal{L}_{\text{CSC}}$ and $\mathcal{L}_{\text{CSV}}$ are the custodial symmetry conserving and violating pieces, respectively. The terms that contribute to $\mathcal{L}_{\text{CSV}}$ reside in the scalar potential, and do not effect the gauge boson mass relation at tree-level. Hence, these terms only contribute a finite correction at one-loop to the T parameter. Nevertheless, the experimental determination of T can place significant constraints on the parameters of the 2HDM scalar potential. In this section, we formulate a basis-independent characterization of custodial symmetry. This will permit a clean basis-independent separation of the custodial symmetry conserving and violating pieces of the Higgs Lagrangian as in eq. (4.1).

4.1. Custodial symmetry of the Higgs Sector

4.1.1. Basis-dependent conditions for custodial symmetry

Conditions for custodial symmetry of the Higgs sector in the 2HDM doublet model has been previous addressed by Pomarol and Vega [7]. Consider the 2HDM scalar potential in a generic basis,

$$\mathcal{V} = m_{11}^2 \Phi_1^\dagger \Phi_1 + m_{22}^2 \Phi_2^\dagger \Phi_2 - [m_{12}^2 \Phi_1^\dagger \Phi_2 + \text{h.c.}] + \tfrac{1}{2}\lambda_1 (\Phi_1^\dagger \Phi_1)^2 + \tfrac{1}{2}\lambda_2 (\Phi_2^\dagger \Phi_2)^2 + \lambda_3 (\Phi_1^\dagger \Phi_1)(\Phi_2^\dagger \Phi_2)$$

$$+ \lambda_4 (\Phi_1^\dagger \Phi_2)(\Phi_2^\dagger \Phi_1) + \left\{ \tfrac{1}{2}\lambda_5 (\Phi_1^\dagger \Phi_2)^2 + \left[\lambda_6 (\Phi_1^\dagger \Phi_1) + \lambda_7 (\Phi_2^\dagger \Phi_2) \right] \Phi_1^\dagger \Phi_2 + \text{h.c.} \right\} , \tag{4.2}$$

where m_{11}^2, m_{22}^2, $\lambda_1, \lambda_2, \lambda_3, \lambda_4 \in \mathbb{R}$ are real parameters, and $m_{12}^2, \lambda_5, \lambda_6, \lambda_7 \in \mathbb{C}$ are potentially complex. The vacuum expectation values of the neutral Higgs fields, denoted by

$$\langle \Phi_a^0 \rangle \equiv \frac{v_a}{\sqrt{2}} \in \mathbb{C} , \qquad a = 1, 2 , \tag{4.3}$$

are also generically complex. Pomarol and Vega asserted that the imposition of custodial symmetry on the 2HDM scalar potential yields two independent cases [in the notation of eq. (4.2)]:

Case 1 : $\quad v_1, v_2 \in \mathbb{R} , \quad \lambda_4 = \lambda_5 , \quad$ and $\quad m_{12}^2, \lambda_5, \lambda_6, \lambda_7 \in \mathbb{R} , \tag{4.4}$

Case 2 : $\quad v_1 = v_2^* \in \mathbb{C} , \quad m_{11}^2 = m_{22}^2 , \quad \lambda_1 = \lambda_2 = \lambda_3 , \quad \lambda_6 = \lambda_7 , \quad$ and $\quad m_{12}^2, \lambda_5, \lambda_6, \lambda_7 \in \mathbb{C} . \tag{4.5}$

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[13] The choice of Higgs mass is dictated by the global Standard Model fit to precision electroweak data [18–20], which suggests that the Higgs mass must lie above but not too far away from the lower Higgs mass bound (at 95% CL) of 114.4 GeV established at LEP [21]. In Ref. [19], a Higgs mass of 117 GeV is chosen for the reference Standard Model in the analysis of new physics contributions to the Peskin-Takeuchi S, T and U parameters.

These conditions are derived as follows.

In Case 1, one constructs two 2×2 matrix fields,[14]

$$M_1 \equiv (\widetilde{\Phi}_1 \,, \Phi_1), \qquad M_2 \equiv (\widetilde{\Phi}_2 \,, \Phi_2), \tag{4.6}$$

where $\widetilde{\Phi} \equiv i\sigma_2 \Phi^*$. The matrix fields transform under $SU(2)_L \times SU(2)_R$ as

$$M_a \to L \, M_a \, R^\dagger \,, \qquad a = 1, 2 \,. \tag{4.7}$$

The $SU(2)_L \times SU(2)_R$ scalar potential is constructed by employing the manifestly invariant combinations, $\text{Tr}[M_1^\dagger M_1]$, $\text{Tr}[M_2^\dagger M_2]$ and $\text{Tr}[M_1^\dagger M_2]$.[15] Explicitly,

$$\mathcal{V} = \tfrac{1}{2} m_{11}^2 \text{Tr}[M_1^\dagger M_1] + \tfrac{1}{2} m_{22}^2 \text{Tr}[M_2^\dagger M_2] - m_{12}^2 \text{Tr}[M_1^\dagger M_2] + \tfrac{1}{8}\lambda_1 \left(\text{Tr}[M_1^\dagger M_1] \right)^2 + \tfrac{1}{8}\lambda_2 \left(\text{Tr}[M_2^\dagger M_2] \right)^2$$

$$+ \tfrac{1}{4}\lambda_3 \text{Tr}[M_1^\dagger M_1] \text{Tr}[M_2^\dagger M_2] + \tfrac{1}{2}\lambda \left(\text{Tr}[M_1^\dagger M_2] \right)^2 + \tfrac{1}{2} \left(\lambda_6 \text{Tr}[M_1^\dagger M_1] + \lambda_7 \text{Tr}[M_2^\dagger M_2] \right) \text{Tr}[M_1^\dagger M_2] \,, \tag{4.8}$$

where hermiticity implies that all the coefficients above are real. Thus, imposing the $SU(2)_L \times SU(2)_R$ symmetry on the scalar potential and comparing with eq. (4.2) then yields $\lambda = \lambda_4 = \lambda_5$ and $m_{12}^2, \lambda_5, \lambda_6, \lambda_7 \in \mathbb{R}$. If the scalar field vacuum expectation values satisfy:

$$\langle M_a \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} v_a^* & 0 \\ 0 & v_a \end{pmatrix} = \frac{v_a}{\sqrt{2}} \mathbb{1}_{2\times 2} \,, \tag{4.9}$$

then $\langle M_a \rangle$ is invariant under the $SU(2)_V$ custodial symmetry group, since $\langle M_a \rangle \to L\langle M_a \rangle R^\dagger = \langle M_a \rangle$ when $L = R$. Eq. (4.9) imposes the condition $v_a \in \mathbb{R}$, and eq. (4.4) is thus established.

In Case 2, one constructs the 2×2 matrix field,

$$M_{12} \equiv (\widetilde{\Phi}_1 \,, \Phi_2), \tag{4.10}$$

which transforms under $SU(2)_L \times SU(2)_R$ as

$$M_{12} \to L \, M_{12} \, R^\dagger \,. \tag{4.11}$$

The $SU(2)_L \times SU(2)_R$ scalar potential is constructed by employing the manifestly invariant combinations $\text{Tr}[M_{12}^\dagger M_{12}]$, $\det M_{12}$, $\det(M_{12})^2$ and $\det[M_{12}^\dagger M_{12}]$. Explicitly,

$$\mathcal{V} = m^2 \text{Tr}[M_{12}^\dagger M_{12}] - \left(m_{12}^2 \det M_{12} + \text{h.c.} \right) + \tfrac{1}{2}\lambda \left(\text{Tr}[M_{12}^\dagger M_{12}] \right)^2$$

$$+ \lambda_4 \det[M_{12}^\dagger M_{12}] + \tfrac{1}{2} \left(\lambda_5 \det(M_{12})^2 + \text{h.c.} \right) + \left(\lambda' \det M_{12} \text{Tr}[M_{12}^\dagger M_{12}] + \text{h.c.} \right) \,. \tag{4.12}$$

Thus, imposing the $SU(2)_L \times SU(2)_R$ symmetry on the scalar potential and comparing with eq. (4.2) then yields $m^2 = m_{11}^2 = m_{22}^2$, $\lambda = \lambda_1 = \lambda_2 = \lambda_3$, $\lambda' = \lambda_6 = \lambda_7$ and $m_{12}^2, \lambda_5, \lambda_6, \lambda_7 \in \mathbb{C}$. If the scalar field vacuum expectation values satisfy:

$$\langle M_{12} \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} v_1^* & 0 \\ 0 & v_2 \end{pmatrix} = \frac{v_2}{\sqrt{2}} \mathbb{1}_{2\times 2} \,, \tag{4.13}$$

then $\langle M_{21} \rangle$ is invariant under the $SU(2)_V$ custodial symmetry group. Eq. (4.13) imposes the condition $v_1^* = v_2 \in \mathbb{C}$, and eq. (4.5) is thus established.

Although the two cases of Pomarol and Vega appear to be distinct, a more careful analysis shows that the two cases are in fact equivalent, and correspond to the formulation of the 2HDM in two different choices of the scalar field basis. This can be established as follows. First, we note that in both Cases 1 and 2, the scalar potential depends on

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[14] In the notation of eq. (4.6), $\widetilde{\Phi}_a$ is the first column and Φ_a is the second column of the matrix M_a (for $a = 1, 2$).

[15] One can check that $\text{Tr}[M_1^\dagger M_2] = \text{Tr}[M_2^\dagger M_1]$ and $\det M_a = \tfrac{1}{2}\text{Tr}[M_a^\dagger M_a]$ (for $a = 1, 2$), so only three independent invariant quadratic forms are relevant.

three independent squared-mass parameters and six independent scalar self-coupling parameters. Now, suppose one begins with a 2HDM subject to the constraints of Case 2 [eq. (4.5)]. It is convenient to define:

$$\widehat{v}_1 = \widehat{v}_2^* = \frac{1}{\sqrt{2}}e^{i\theta}\,, \qquad m^2 \equiv m_{11}^2 = m_{22}^2\,, \qquad \lambda \equiv \lambda_1 = \lambda_2 = \lambda_3\,, \qquad \lambda' \equiv \lambda_6 = \lambda_7\,, \tag{4.14}$$

where $\widehat{v}_a$ is defined in eq. (2.3). By performing a basis transformation, $\Phi_a \to U_{a\bar{b}}\Phi_b$, with

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta} & e^{i\theta} \\ -ie^{-i\theta} & ie^{i\theta} \end{pmatrix}\,, \tag{4.15}$$

the coefficients of the scalar potential [cf. eq. (4.2)] are transformed to [in the notation of eq. (2.8)]:

$$Y_1 = m^2 - \mathrm{Re}(m_{12}^2 e^{-2i\theta})\,, \tag{4.16}$$

$$Y_2 = m^2 + \mathrm{Re}(m_{12}^2 e^{-2i\theta})\,, \tag{4.17}$$

$$Y_3 = -\mathrm{Im}(m_{12}^2 e^{-2i\theta})\,, \tag{4.18}$$

$$Z_1 = \lambda + \tfrac{1}{2}\lambda_4 + \tfrac{1}{2}\mathrm{Re}(\lambda_5 e^{-4i\theta}) + 2\mathrm{Re}(\lambda' e^{-2i\theta})\,, \tag{4.19}$$

$$Z_2 = \lambda + \tfrac{1}{2}\lambda_4 + \tfrac{1}{2}\mathrm{Re}(\lambda_5 e^{-4i\theta}) - 2\mathrm{Re}(\lambda' e^{-2i\theta})\,, \tag{4.20}$$

$$Z_3 = \lambda - \tfrac{1}{2}\lambda_4 - \tfrac{1}{2}\mathrm{Re}(\lambda_5 e^{-4i\theta})\,, \tag{4.21}$$

$$Z_4 = Z_5 = \tfrac{1}{2}\lambda_4 - \tfrac{1}{2}\mathrm{Re}(\lambda_5 e^{-4i\theta})\,, \tag{4.22}$$

$$Z_6 = \tfrac{1}{2}\mathrm{Im}(\lambda_5 e^{-4i\theta}) + \mathrm{Im}(\lambda' e^{-2i\theta})\,, \tag{4.23}$$

$$Z_7 = -\tfrac{1}{2}\mathrm{Im}(\lambda_5 e^{-4i\theta}) + \mathrm{Im}(\lambda' e^{-2i\theta})\,, \tag{4.24}$$

while the normalized scalar field vacuum expectation values are transformed to:

$$\widehat{v}_a \longrightarrow U_{a\bar{b}}\widehat{v}_b = \delta_{a1}\,. \tag{4.25}$$

Eq. (4.25) defines the Higgs basis $\{H_1\,, H_2\}$, up to a phase redefinition of H_2. We immediately note that $Z_4 = Z_5$ and the vacuum expectation values and all the scalar potential parameters are real. Thus, the Higgs basis satisfies all the conditions of Case 1 of Pomarol and Vega [cf. eq. (4.4)]. Moreover, it is easy to check that any additional O(2) basis transformation preserves $\lambda_4 = \lambda_5$ and the reality of the scalar potential parameters. Thus, we have confirmed that Cases 1 and 2 of Pomarol and Vega are equivalent and simply represent different choices of the scalar field basis.[16]

Of course, one can also perform arbitrary U(2) transformations of the Higgs fields. The resulting scalar potential parameters and vacuum expectation values will in general satisfy neither case 1 nor case 2 of Pomarol and Vega. Yet, all these parameterizations are physically equivalent and maintain the custodial symmetry. Clearly, it is desirable to formulate a basis-independent description of custodial symmetry. We shall provide such a formulation in the next subsection.

4.1.2. The Basis-Independent Condition for Custodial Symmetry in the Scalar Sector

It is possible generalize the two implementations of custodial symmetry presented in the previous subsection by constructing an $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$ invariant scalar potential using the Higgs basis fields, H_1 and H_2. The advantage of this basis choice is that no supplementary conditions on the vevs are required. In particular, we define 2×2 matrix fields:

$$\mathsf{M}_1 \equiv (\widetilde{H}_1\,, H_1), \quad \mathsf{M}_2 \equiv (\widetilde{H}_2\,, H_2), \quad \mathsf{M}_{12} \equiv (\widetilde{H}_1\,, H_2), \quad \mathsf{M}_{21} \equiv (\widetilde{H}_2\,, H_1)\,. \tag{4.26}$$

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[16] In ref. [22], it was shown that in Type-I and Type-II 2HDMs, the corresponding Higgs-fermion Yukawa couplings (defined in the standard basis where the discrete symmetry $\Phi_2 \to -\Phi_2$ is manifest) are custodial symmetric if and only if the scalar potential parameters satisfy eqs. (4.4) and (4.5), respectively. The two ways to implement custodial symmetry given by eqs. (4.7) and (4.11), respectively, can be distinguished based on the presence or absence of the $A^0 GG$ effective interaction. This is possible, as the special forms of the Type I and II Higgs-Yukawa interactions effectively select a "preferred" basis.

Since $\langle H_1^0 \rangle = v/\sqrt{2}$ (where $v = 246$ GeV) and $\langle H_2^0 \rangle = 0$, it follows that

$$\langle \mathbb{M}_1 \rangle = \frac{v}{\sqrt{2}} \mathbb{1}_{2\times 2}, \qquad \langle \mathbb{M}_2 \rangle = 0, \tag{4.27}$$

whereas neither $\langle \mathbb{M}_{12} \rangle$ nor $\langle \mathbb{M}_{21} \rangle$ are proportional to the identity matrix. Consequently, if we wish to preserve a custodial $SU(2)_V$ after electroweak symmetry breaking, the scalar potential in the Higgs basis *must* be solely a function of $\mathbb{M}_1$ and $\mathbb{M}_2$.

In the Higgs basis, the field H_1 is basis-invariant, as it is defined such that $\langle H_1^0 \rangle \equiv v/\sqrt{2}$ is real and positive. On the other hand, since $\langle H_2^0 \rangle = 0$ it follows that H_2 is only defined up to an overall rephasing. That is, H_1 is an invariant field with respect to basis transformations, whereas H_2 is a pseudo-invariant field. As a result, the $SU(2)_L \times SU(2)_R$ transformation laws for $\mathbb{M}_1$ and $\mathbb{M}_2$ are given by:

$$\mathbb{M}_1 \to L\,\mathbb{M}_1 R^\dagger, \qquad \mathbb{M}_2 \to L\,\mathbb{M}_2 R'^\dagger, \qquad L \in SU(2)_L, \quad R,\, R' \in SU(2)_R. \tag{4.28}$$

Since H_i and $\widetilde{H}_i$ ($i = 1,2$) are doublets under the weak $SU(2)_L$ gauge transformation, the transformation matrices L appearing in eq. (4.28) must be the same in the $SU(2)_L \times SU(2)_R$ transformation laws of $\mathbb{M}_1$ and $\mathbb{M}_2$. As noted by [16], the same requirement does not hold for the $SU(2)_R$ transformation; hence in general $R' \neq R$. However, R and R' are related by the fact that the gauged $U(1)$ hypercharge operator, $Y \equiv \mathrm{diag}(-1\,,\,+1)$, is a diagonal generator of $SU(2)_R$. In particular, if we write $R \equiv \exp(i\theta n^a T_R^a)$ where (n^1, n^2, n^3) is a unit vector, then T_R^3 is proportional to Y. Since the H_i are hypercharge $+1$ fields and the $\widetilde{H}_i$ are hypercharge -1 fields, the relation between R and R' is fixed by $R' \equiv PRP^{-1}$, where P is an $SU(2)$ matrix and $P \exp(i\theta Y) P^{-1} = \exp(i\theta Y)$ for all θ [16]. By expanding in θ, it follows that $PY = YP$, which constrains P to be of the form $P = \mathrm{diag}(e^{-i\chi}\,,\, e^{i\chi})$, where $0 \leq \chi < 2\pi$. We conclude that the most general form for the $SU(2)_L \times SU(2)_R$ transformation laws for $\mathbb{M}_1$ and $\mathbb{M}_2$ is given by

$$\mathbb{M}_1 \to L\,\mathbb{M}_1 R^\dagger, \qquad \mathbb{M}_2 \to L\,\mathbb{M}_2 P R^\dagger P^{-1}, \tag{4.29}$$

where

$$L \in SU(2)_L, \quad R \in SU(2)_R, \qquad P \equiv \begin{pmatrix} e^{-i\chi} & 0 \\ 0 & e^{i\chi} \end{pmatrix}, \quad (0 \leq \chi < 2\pi). \tag{4.30}$$

The phase angle χ can be interpreted as representing the freedom to rephase the field H_2. In particular, if one defines $\mathbb{M}_1' \equiv \mathbb{M}_1$ and $\mathbb{M}_2' \equiv \mathbb{M}_2 P$, then the transformation laws for $\mathbb{M}_1'$ and $\mathbb{M}_2'$ are the same, i.e. $\mathbb{M}_a' \to L\,\mathbb{M}_a' R^\dagger$ for $a = 1, 2$.

The $SU(2)_L \times SU(2)_R$ scalar potential is constructed by employing the manifestly invariant combinations, $\mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_1]$, $\mathrm{Tr}[\mathbb{M}_2^\dagger \mathbb{M}_2]$ and $\mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_2 P]$.[17] Explicitly,

$$\mathcal{V} = \tfrac{1}{2} Y_1 \mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_1] + \tfrac{1}{2} Y_2 \mathrm{Tr}[\mathbb{M}_2^\dagger \mathbb{M}_2] + \widetilde{Y}_3 \mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_2 P] + \tfrac{1}{8} Z_1 \left(\mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_1] \right)^2 + \tfrac{1}{8} Z_2 \left(\mathrm{Tr}[\mathbb{M}_2^\dagger \mathbb{M}_2] \right)^2$$

$$+ \tfrac{1}{4} Z_3 \mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_1] \mathrm{Tr}[\mathbb{M}_2^\dagger \mathbb{M}_2] + \tfrac{1}{2} \lambda \left(\mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_2 P] \right)^2 + \tfrac{1}{2} \left(\widetilde{Z}_6 \mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_1] + \widetilde{Z}_7 \mathrm{Tr}[\mathbb{M}_2^\dagger \mathbb{M}_2] \right) \mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_2 P], \tag{4.31}$$

where hermiticity implies that all coefficients above are real. Eq. (4.31) is equivalent to

$$\mathcal{V} = Y_1 H_1^\dagger H_1 + Y_2 H_2^\dagger H_2 + [Y_3 H_1^\dagger H_2 + \mathrm{h.c.}]$$

$$+ \tfrac{1}{2} Z_1 (H_1^\dagger H_1)^2 + \tfrac{1}{2} Z_2 (H_2^\dagger H_2)^2 + Z_3 (H_1^\dagger H_1)(H_2^\dagger H_2) + Z_4 (H_1^\dagger H_2)(H_2^\dagger H_1)$$

$$+ \left\{ \tfrac{1}{2} Z_5 (H_1^\dagger H_2)^2 + \left[Z_6 (H_1^\dagger H_1) + Z_7 (H_2^\dagger H_2) \right] H_1^\dagger H_2 + \mathrm{h.c.} \right\}, \tag{4.32}$$

where

$$\widetilde{Y}_3 = Y_3 e^{-i\chi} = Y_3^* e^{i\chi} \in \mathbb{R}, \qquad \lambda = Z_4 = Z_5 e^{-2i\chi} = Z_5^* e^{2i\chi} \in \mathbb{R},$$

$$\widetilde{Z}_6 = Z_6 e^{-i\chi} = Z_6^* e^{i\chi} \in \mathbb{R}, \qquad \widetilde{Z}_7 = Z_7 e^{-i\chi} = Z_7^* e^{i\chi} \in \mathbb{R}. \tag{4.33}$$

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[17] Note that $\mathrm{Tr}[\mathbb{M}_1^\dagger \mathbb{M}_2 P] = \mathrm{Tr}[\mathbb{M}_2^\dagger \mathbb{M}_1 P^{-1}]$, so only three independent invariant quadratic forms are possible.

Eq. (4.33) implies that:

$$\text{Im}(Y_3 e^{-i\chi}) = \text{Im}(Z_5 e^{-2i\chi}) = \text{Im}(Z_6 e^{-i\chi}) = \text{Im}(Z_7 e^{-i\chi}) = 0 , \qquad (4.34)$$

which immediately implies that the scalar potential is CP-conserving. Hence according to eq. (4.33), the conditions for custodial symmetry are given by

$$Z_4 = Z_5 e^{-2i\chi} \in \mathbb{R} , \qquad Z_6 e^{-i\chi} , \; Z_7 e^{-i\chi} \in \mathbb{R} . \qquad (4.35)$$

Note that the conditions of eq. (4.35) are basis-independent. In particular, under a basis transformation $\Phi_a \to U_{a\bar{b}} \Phi_b$,

$$e^{i\chi} \to (\det U)^{-1} e^{i\chi} . \qquad (4.36)$$

In the case of $Z_6 \neq 0$ and/or $Z_7 \neq 0$, one can relate the angle χ to θ_{23}. In particular, by comparing eqs. (3.4) and (4.34) it follows that $e^{-i\chi} = \pm \eta e^{-i\theta_{23}}$. The $\pm$ ambiguity is removed by squaring this result, which yields

$$e^{-2i\chi} = \eta^2 e^{-2i\theta_{23}} . \qquad (4.37)$$

The phase η^2 is specified in Tables II and VI for the various cases under which CP conservation holds. In general, the basis-independent condition for custodial symmetry is:

$$Z_4 = \eta^2 \text{Re}(Z_5 e^{-2i\theta_{23}}) , \qquad (4.38)$$

where we have used the fact that $\text{Im}(Z_5 e^{-2i\theta_{23}}) = 0$ for a CP-conserving 2HDM scalar potential.[18]
  One can also eliminate the phase angle χ using eq. (4.33):

$$e^{-2i\chi} = \frac{Z_6^*}{Z_6} = \frac{Z_7^*}{Z_7} . \qquad (4.39)$$

Consequently, if $Z_6 \neq 0$ then eq. (4.35) is equivalent to[19]

$$Z_4 = \frac{Z_5 Z_6^{*2}}{|Z_6|^2} = \varepsilon_{56} |Z_5| , \qquad (4.40)$$

where the invariant quantity ε_{56} was introduced initially in eq. (3.12). The condition for custodial symmetry given by eq. (4.40) is manifestly basis-independent.[20] Similarly, if $Z_7 \neq 0$, the basis-independent condition for custodial symmetry can be written in the following form:

$$Z_4 = \frac{Z_5 Z_7^{*2}}{|Z_7|^2} = \varepsilon_{57} |Z_5| , \qquad (4.41)$$

where the invariant quantity ε_{57} was introduced initially in eq. (3.21). Finally, if $\rho^Q \neq 0$, then under the assumption that $Z_6 \neq 0$ and/or $Z_7 \neq 0$, one can use eqs. (3.31) and (4.38) to obtain:[21]

$$Z_4 = \varepsilon_{5Q} |Z_5| . \qquad (4.42)$$

In the real Higgs basis, defined as the basis in which the scalar potential parameters and the Yukawa coupling matrices ρ^Q are simultaneously real, ε_{56}, ε_{57} and ε_{5Q} coincide with the sign of Z_5. Thus eqs. (4.40), (4.41) and (4.42) reduce to the simple relation, $Z_4 = Z_5$, in the real Higgs basis. This result is consistent with eq. (4.22) obtained previously. Note that the condition $Z_4 = Z_5$ is invariant with respect to $H_2 \to -H_2$, which is the only remaining basis freedom within the real basis.
  The special case of $Z_6 = Z_7 = 0$ must be treated separately. In this case, $Y_3 = 0$ by virtue of eq. (2.15) and Z_5 is the only potentially complex parameter of the scalar potential in the Higgs basis. The condition for a custodial symmetric scalar potential is now given by the single condition, $Z_4 = Z_5 e^{-2i\chi} \in \mathbb{R}$ [cf. eq. (4.35)]. Writing $Z_5 = |Z_5| e^{2i\theta_5}$, it

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[18] For Case III$'$ of Table VI, one must replace θ_{23} and η^2 with $\bar{\theta}_{23}$ and $\bar{\eta}^2$, respectively [cf. eq. (3.18)].
[19] CP conservation requires that $\text{Im}(Z_5 Z_6^{*2}) = \text{Im}(Z_5 Z_7^{*2}) = 0$. Hence the numerators of eqs. (4.40) and (4.41) are manifestly real, as required since Z_4 is a real parameter.
[20] Eq. (4.40) can also be obtained from eqs. (3.15) and (4.38), after noting that $\eta^4 = 1$.
[21] In deriving eq. (4.42) we used the fact that $\eta^4 = 1$ in Cases I$'$ and II$'$, and $\bar{\eta}^4 = 1$ in Case III$'$

follows that $\theta_5 + \chi = n\pi/2$ for some integer n. That is, the basis-independent condition for custodial symmetry is given simply by:

$$Z_4 = \pm|Z_5|\,. \tag{4.43}$$

In contrast to eqs. (4.40), (4.41) and (4.42), where Z_4 is uniquely determined (and is equal to Z_5 in the real Higgs basis), in the special case of $Z_6 = Z_7 = 0$, there are two solutions for Z_4 that are consistent with a custodial symmetric scalar potential. This result can also be deduced by noting that when $Z_6 = Z_7 = 0$, eqs. (3.4) and (4.34) yield $e^{-2i\chi} = \pm\eta e^{-2i\theta_{23}}$, where the $\pm$ ambiguity cannot be removed [in contrast to eq. (4.37)]. Hence, when $Z_6 = Z_7 = 0$, the basis-independent condition for custodial symmetry is [cf. footnote 18]:

$$Z_4 = \pm\eta^2 \mathrm{Re}(Z_5 e^{-2i\theta_{23}})\,, \tag{4.44}$$

which again exhibits two possible solutions. Since $\eta^2 = \pm 1$ and $\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$, eq. (4.44) is equivalent to eq. (4.43) as expected.

The above results do not depend on the Yukawa coupling matrix ρ^Q. If $\rho^Q = 0$, then one is free to redefine $H_2 \to iH_2$, which has the effect of transforming $Z_5 \to -Z_5$. In this case, the sign of Z_5 in the real Higgs basis is basis-dependent, and the two conditions $Z_4 = \pm Z_5$ are equivalent. Nevertheless, there are still two solutions for Z_4 since a custodial symmetric scalar potential is possible with either sign for Z_4. If $\rho^Q \neq 0$, then the transformation $H_2 \to iH_2$ has the effect of transforming ρ^Q to $i\rho^Q$. If the neutral Higgs–fermion interactions are CP-conserving, then a real Higgs basis exists in which Z_5 and ρ^Q are simultaneously real. In this case, the sign of Z_5 in the real Higgs basis is meaningful. In contrast to eq. (4.42), the condition for a custodial symmetric scalar potential, which can be obtained directly from eqs. (3.31) and (4.44), is given by:

$$Z_4 = \pm\varepsilon_{5Q}|Z_5|\,. \tag{4.45}$$

The existence of these two possible solutions when $Z_6 = Z_7 = 0$ has a critical impact on the nature of the Higgs mass degeneracy in the custodial limit, as shown in the next subsection. If the neutral Higgs–fermion interactions are CP-violating, then ε_{5Q} has no meaning and eq. (4.45) must be discarded. Nevertheless, the conclusion that $Z_4 = \pm|Z_5|$ for a custodial symmetric scalar potential with $Z_6 = Z_7 = 0$ still applies.

In summary, the basis-independent condition for a custodial-symmetric scalar potential is given by:

$$Z_4 = \begin{cases} \varepsilon_{56}|Z_5|\,, & \text{for } Z_6 \neq 0\,, \\ \varepsilon_{57}|Z_5|\,, & \text{for } Z_7 \neq 0\,, \\ \pm|Z_5|\,, & \text{for } Z_6 = Z_7 = 0\,. \end{cases} \tag{4.46}$$

The above conditions do not depend on the form of the neutral Higgs–fermion interactions. However, if the neutral Higgs–fermion interactions are CP-conserving, then there exists an invariant quantity ε_{5Q}, defined in eq. (3.29), which is equal to the sign of Z_5 in the real Higgs basis (where all scalar potential parameters and ρ^Q are real). In this case, we also have

$$Z_4 = \begin{cases} \varepsilon_{5Q}|Z_5|\,, & \text{for } Z_6 \neq 0 \text{ and/or } Z_7 \neq 0\,, \\ \pm\varepsilon_{5Q}|Z_5|\,, & \text{for } Z_6 = Z_7 = 0\,. \end{cases} \tag{4.47}$$

In a real Higgs basis, the general condition for a custodial symmetric scalar potential is $Z_4 = Z_5$. In the special case of $Z_6 = Z_7 = 0$, the condition $Z_4 = -Z_5$ also yields a custodial symmetric scalar potential. These two conditions are physically inequivalent when $\rho^Q \neq 0$.

4.1.3. Higgs mass degeneracy in the custodial limit

The squared-mass of the charged Higgs boson is given by eq. (2.22). If $Z_6 \neq 0$ and/or $Z_7 \neq 0$ and if CP is conserved in the neutral Higgs sector, then the squared-mass of the CP-odd Higgs boson is given by eqs. (3.17) and (3.26), which we can rewrite as:

$$m_{A^0}^2 = \begin{cases} m_{H^\pm}^2 + \frac{1}{2}v^2(Z_4 - \varepsilon_{56}|Z_5|)\,, & \text{if } Z_6 \neq 0\,, \\ m_{H^\pm}^2 + \frac{1}{2}v^2(Z_4 - \varepsilon_{57}|Z_5|)\,, & \text{if } Z_7 \neq 0\,. \end{cases} \tag{4.48}$$

In the custodial limit eq. (4.46) applies, and it follows that

$$m_{H^\pm}^2 = m_{A^0}^2 = Y_2 + \tfrac{1}{2}Z_3 v^2 \,, \tag{4.49}$$

in agreement with the results of [7]. That is, the charged Higgs boson and the CP-odd Higgs boson are mass-degenerate in the custodial limit.

The case of $Z_6 = Z_7 = 0$ is special, as discussed in Section 3.3. In this case, there is one neutral CP-even Higgs boson, denoted by h_1^0, with squared-mass $m_{h_1^0}^2 = Z_1 v^2$ and two neutral Higgs states of indeterminate CP quantum number, denoted by h_2^0 and h_3^0, with squared-masses given by eq. (3.28), which yields:

$$m_{h_2^0, h_3^0}^2 = m_{H^\pm}^2 + \tfrac{1}{2}v^2 (Z_4 \mp |Z_5|) \,. \tag{4.50}$$

According to eq. (4.46), $Z_4 = \pm|Z_5|$ in the custodial limit. We conclude that either one of the states h_2^0 or h_3^0 can be degenerate in mass with the charged Higgs boson. However, the CP-quantum number of h_2^0 and h_3^0 are indeterminate (if the Higgs-fermion interactions are neglected), since there are two inequivalent definitions of CP when $Z_6 = Z_7 = 0$. This ambiguity can be resolved if the neutral Higgs-fermion interactions are CP-conserving.[22] In this case, the two neutral states can be identified as a CP-even state h^0 or H^0 and a CP-odd state A^0. Using eqs. (4.47) and (3.28), it follows that:

$$m_{H^\pm}^2 = \begin{cases} m_{A^0}^2 & \text{if } Z_4 = \varepsilon_{5Q}|Z_5| \quad \text{and} \quad Z_6 = Z_7 = 0 \,, \\ m_{h^0}^2 & \text{if } Z_4 = -\varepsilon_{5Q}|Z_5| \,, \quad m_{H^\pm}^2 < Z_1 v^2 \quad \text{and} \quad Z_6 = Z_7 = 0 \,, \\ m_{H^0}^2 & \text{if } Z_4 = -\varepsilon_{5Q}|Z_5| \,, \quad m_{H^\pm}^2 > Z_1 v^2 \quad \text{and} \quad Z_6 = Z_7 = 0 \,. \end{cases} \tag{4.51}$$

where $m_{H^0} > m_{h^0}$ by convention. In particular, $m_{H^\pm}^2 = m_{A^0}^2$ if $Z_4 = Z_5$ in the real Higgs basis, whereas $m_{H^\pm}^2 = m_{H^0}^2$ if $Z_4 = -Z_5$ in the real Higgs basis. This result is easy to understand. If $Z_4 = -Z_5$, we can perform a basis transformation $H_2 \to iH_2$, which yields $Z_4 = Z_5$ and $\rho^Q \to i\rho^Q$. The effect of the latter is to transform the pseudoscalar Yukawa coupling of the neutral Higgs boson into a scalar Yukawa coupling. The case in which the charged Higgs boson is mass-degenerate with the CP-even neutral Higgs boson corresponds to the case of "twisted custodial symmetry" introduced in [16].

Although this final conclusion is the same, we disagree with the interpretation of "twisted custodial symmetry" given in ref. [16]. As employed in ref. [16], the term "twisted" is associated with a particular choice of the angle χ in the $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$ transformation law of $\mathbb{M}_2$ given in eq. (4.29). However, we have shown above that this angle is basis-dependent and thus has no physical significance. It is also argued in ref. [16] that custodial symmetry plays a critical role in formulating the "twisted" scenario. We have shown above that the "twisted" scenario is a consequence of the two-fold ambiguity in the definition of CP in the special case of $Z_6 = Z_7 = 0$ (in the absence of the Higgs–fermion Yukawa couplings). This ambiguity exists whether or not the custodial symmetry is present, as shown in Section 3.3. The custodial symmetry is relevant in the following sense. The possibility that $m_{H^\pm}^2 = m_{h^0}^2$ or $m_{H^\pm}^2 = m_{H^0}^2$ arises precisely because the custodial symmetry condition $Z_4 = \pm \varepsilon_{5Q}|Z_5|$ allows for a negative sign in this relation if and only if $Z_6 = Z_7 = 0$.

4.2. Custodial symmetry in the Higgs-fermion sector for the general 2HDM

We now examine the Higgs-fermion Yukawa interactions in more detail, and discuss the implications of custodial symmetry for this sector.

Custodial symmetry in the Yukawa Lagrangian was analyzed for the Type I and II 2HDM in [22]. Here we will shall examine the general 2HDM without assuming additional conditions to restrict the terms of the Higgs–fermion Yukawa Lagrangian. In a generic basis, the Higgs-fermion Lagrangian is given by eq. (2.24). It is convenient to rewrite this Lagrangian in the following compact form:

$$-\mathscr{L}_Y = \overline{\mathcal{Q}}_L \widetilde{\Phi}_{\bar{a}} \eta_a^U \mathcal{U}_R + \overline{\mathcal{Q}}_L \Phi_a \eta_{\bar{a}}^{D\,\dagger} D_R + \text{h.c.} \,, \tag{4.52}$$

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[22] If the neutral Higgs–fermion interactions are CP-violating, then the neutral Higgs state that is degenerate in mass with the charged Higgs boson does not possess a well-defined CP quantum number.

where $\mathcal{U} \equiv K^\dagger U$, $\overline{\mathcal{Q}}_L \equiv (\overline{\mathcal{U}} \ \overline{\mathcal{D}})_L$, and $\Phi_a \equiv \begin{pmatrix} \Phi_a^+ \\ \Phi_a^0 \end{pmatrix}$. In the Higgs basis, the corresponding Lagrangian given in eq. (2.26) can likewise be expressed compactly as:

$$-\mathscr{L}_Y = \overline{\mathcal{Q}}_L(\widetilde{H}_1\kappa^U + \widetilde{H}_2\rho^U)\mathcal{U}_R + \overline{\mathcal{Q}}_L(H_1\kappa^{D\,\dagger} + H_2\rho^{D\,\dagger})D_R + \text{h.c.}\,, \tag{4.53}$$

where the basis-invariant coupling matrices κ^Q and ρ^Q are defined in eq. (2.25).

4.2.1. Basis-dependent formulation of custodial symmetry in the Higgs–fermion sector

We first examine the conditions for custodial symmetry of the Higgs-fermion Yukawa interactions in the two basis choices of Pomarol and Vega following the results of Section 4.1.1. In Case 1, one writes the Yukawa interactions in terms of the 2×2 matrix fields M_1 and M_2 defined in eq. (4.6). The form of the Yukawa interactions invariant under $SU(2)_L \times SU(2)_R$ is then given by:

$$-\mathscr{L}_Y = \eta_1\overline{\mathcal{Q}}_L \ M_1 \begin{pmatrix} \mathcal{U}_R \\ D_R \end{pmatrix} + \eta_2\overline{\mathcal{Q}}_L \ M_2 \begin{pmatrix} \mathcal{U}_R \\ D_R \end{pmatrix} + \text{h.c.}\,, \tag{4.54}$$

One can easily check that eq. (4.54) is manifestly invariant under the $SU(2)_L \times SU(2)_R$ transformations

$$M_i \to LM_iR^\dagger\,, \qquad \overline{\mathcal{Q}}_L \to \overline{\mathcal{Q}}_LL^\dagger\,, \qquad \begin{pmatrix} \mathcal{U}_R \\ D_R \end{pmatrix} \to R\begin{pmatrix} \mathcal{U}_R \\ D_R \end{pmatrix}. \tag{4.55}$$

Comparing with eq. (4.52) then yields the custodial symmetry conditions,

$$\eta_1 = \eta_1^U = \eta_1^{D\dagger}\,, \qquad \eta_2 = \eta_2^U = \eta_2^{D\dagger}\,. \tag{4.56}$$

In Case 2, one writes the Yukawa interactions in terms of the 2×2 matrix fields

$$M_{12} \equiv (\widetilde{\Phi}_1\,, \Phi_2)\,, \qquad M_{21} \equiv (\widetilde{\Phi}_2\,, \Phi_1)\,, \tag{4.57}$$

which transforms under $SU(2)_L \times SU(2)_R$ as

$$M_{12} \to L \ M_{12} \ R^\dagger\,, \qquad M_{21} \to L \ M_{21} \ R^\dagger\,. \tag{4.58}$$

The form of the Yukawa interactions invariant under $SU(2)_L \times SU(2)_R$ is then given by:

$$-\mathscr{L}_Y = \eta_{12}\overline{\mathcal{Q}}_L \ M_{12} \begin{pmatrix} \mathcal{U}_R \\ D_R \end{pmatrix} + \eta_{21}\overline{\mathcal{Q}}_L \ M_{21} \begin{pmatrix} \mathcal{U}_R \\ D_R \end{pmatrix} + \text{h.c.}\,. \tag{4.59}$$

Comparing with eq. (4.52) then yields the custodial symmetry conditions,

$$\eta_{12} = \eta_1^U = \eta_2^{D\dagger}\,, \qquad \eta_{21} = \eta_2^U = \eta_1^{D\dagger}\,. \tag{4.60}$$

As in Section 4.1.1, we can demonstrate that Cases 1 and 2 are equivalent and simply represent different choices of the scalar field basis. To prove this assertion, we start from the basis of Case 2 and perform the basis transformation to the Higgs basis as specified by the unitary matrix given by eq. (4.15). Then, κ^Q, ρ^Q are related to the Yukawa coupling matrices η_1^Q, η_2^Q via

$$\begin{pmatrix} \kappa^Q \\ \rho^Q \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta} & e^{i\theta} \\ -ie^{-i\theta} & ie^{i\theta} \end{pmatrix} \begin{pmatrix} \eta_1^Q \\ \eta_2^Q \end{pmatrix}. \tag{4.61}$$

Using the Case 2 custodial symmetry conditions given in eq. (4.60), it follows that:[23]

$$\kappa^U = \frac{1}{\sqrt{2}} \left(e^{i\theta}\eta_2^U + e^{-i\theta}\eta_1^U\right) = \kappa^{D\,\dagger}\,, \tag{4.62}$$

$$\rho^U = \frac{i}{\sqrt{2}} \left(e^{i\theta}\eta_2^U - e^{-i\theta}\eta_1^U\right) = \rho^{D\,\dagger}\,. \tag{4.63}$$

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[23] Using eq. (2.25) with $\widehat{v}_1 = \widehat{v}_2^* = \frac{1}{\sqrt{2}}\,e^{i\theta}$, one immediately reproduces eq. (4.62). The corresponding result for ρ^Q differs by an overall factor of i. But, we are free to redefine the Higgs-basis field $H_2 \to iH_2$, which yields $\rho^Q \to i\rho^Q$ in agreement with eq. (4.63).

That is, in the Higgs basis, the Case 1 custodial symmetry conditions given by eq. (4.56) are satisfied. Moreover, these conditions are preserved under any additional O(2) basis transformation. Thus, we have verified that Cases 1 and 2 of Pomarol and Vega, including the $SU(2)_L \times SU(2)_R$ Higgs–fermion Yukawa interactions specified above, are equivalent and simply represent different choices of the scalar field basis.

Using eq. (2.28), the condition $\kappa^U = \kappa^{D\,\dagger}$ is equivalent to the equality of the up and down-type fermion mass matrices,

$$M_U = M_D \,, \tag{4.64}$$

which is clearly a basis-independent condition. However, the condition $\rho^U = \rho^{D\,\dagger}$ is not quite basis-independent, as ρ^Q is a pseudo-invariant quantity. At this stage, eq. (4.63) has been obtained in a real Higgs basis. In the next subsection, we obtain the basis-independent conditions for custodial symmetry of the Higgs–fermion Yukawa interactions.

4.2.2. Basis-independent formulation of custodial symmetry in the Higgs–fermion sector

Following Section 4.1.2, we introduce the 2×2 matrix fields in the Higgs basis, denoted by $\mathbb{M}_1$ and $\mathbb{M}_2$ [cf. eq. (4.26)], whose transformation properties under $SU(2)_L \times SU(2)_R$ are given by eqs. (4.29) and (4.30). Note that the transformation law for $\mathbb{M}_2$ includes a phase angle degree of freedom χ that reflects the freedom to rephase the Higgs-basis field H_2. The form of the Yukawa interactions invariant under $SU(2)_L \times SU(2)_R$ is then given by:

$$-\mathscr{L}_Y = \kappa\,\overline{\mathcal{Q}}_L\,\mathbb{M}_1\,\begin{pmatrix}\mathcal{U}_R\\D_R\end{pmatrix} + \rho\,\overline{\mathcal{Q}}_L\,\mathbb{M}_2 P\begin{pmatrix}\mathcal{U}_R\\D_R\end{pmatrix} + \text{h.c.}\,, \tag{4.65}$$

where $P \equiv \text{diag}(e^{-i\chi}, e^{i\chi})$. Comparing with eq. (4.53) yields,

$$\kappa = \kappa^U = \kappa^{D\,\dagger}\,, \qquad \rho = e^{i\chi}\rho^U = e^{-i\chi}\rho^{D\,\dagger}\,. \tag{4.66}$$

The first condition above implies $M_U = M_D$, which reproduces the result of eq. (4.64). The second condition is basis independent in light of eqs. (2.27) and (4.36).

For a generic custodial-symmetric Higgs–fermion Yukawa interaction, the matrices ρ^U and ρ^D are correlated according to eq. (4.66), but they can be non-diagonal and complex. Thus, the custodial symmetry does not imply CP-conserving neutral Higgs–fermion couplings. However, we can impose CP-conservation of the neutral Higgs-fermion interactions if the conditions listed in eq. (3.2) are respected. An equivalent set of conditions (which are more useful as they do not rely on Z_5, Z_6 and Z_7) is given by eq. (3.5). In this case, it is convenient to use eq. (4.37) to rewrite the second condition of eq. (4.66) as follows,[24]

$$e^{i\theta_{23}}\rho^U = \eta^2[e^{i\theta_{23}}\rho^D]^\dagger\,, \tag{4.67}$$

which is manifestly basis-independent. The sign factor η^2 is given in Tables II and VI. If $Z_6 = Z_7 = 0$, then Table VI applies with $Z_7 e^{-i\theta_{23}}$ replaced by $\rho^Q e^{i\theta_{23}}$ ($Q = U, D$). In particular, note that for a CP-conserving Higgs–fermion interaction, $\text{Im}(\rho^U e^{i\theta_{23}}) = \text{Im}(\rho^D e^{i\theta_{23}}) = 0$ if $\eta = +1$ and $\text{Re}(\rho^U e^{i\theta_{23}}) = \text{Re}(\rho^D e^{i\theta_{23}}) = 0$ if $\eta = -1$.

5. THE OBLIQUE PARAMETERS S, T AND U

The S, T, and U parameters, introduced by Peskin and Takeuchi [8], are independent ultraviolet-finite combinations of radiative corrections to gauge boson two-point functions (the so-called "oblique" corrections). The parameter T is related to the well known ρ-parameter of electroweak physics [23] by $\rho - 1 = \alpha T$. The oblique parameters can be

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[24] As usual, in Case III$'$ of Table VI, one must replace θ_{23} and η^2 with $\overline{\theta}_{23}$ and $\overline{\eta}^2$, respectively [cf. eq. (3.18)].

expressed in terms of the transverse part of the gauge boson two-point functions [19, 24]:[25]

$$\overline{\alpha}\, T \equiv \frac{\Pi_{WW}^{\text{new}}(0)}{m_W^2} - \frac{\Pi_{ZZ}^{\text{new}}(0)}{m_Z^2}\,, \tag{5.1}$$

$$\frac{\overline{\alpha}}{4\overline{s}_Z^2\overline{c}_Z^2}\, S \equiv \frac{\Pi_{ZZ}^{\text{new}}(m_Z^2) - \Pi_{ZZ}^{\text{new}}(0)}{m_Z^2} - \left(\frac{\overline{c}_W^2 - \overline{s}_W^2}{\overline{c}_W \overline{s}_W}\right)\frac{\Pi_{Z\gamma}^{\text{new}}(m_Z^2)}{m_Z^2} - \frac{\Pi_{\gamma\gamma}^{\text{new}}(m_Z^2)}{m_Z^2}\,, \tag{5.2}$$

$$\frac{\overline{\alpha}}{4\overline{s}_Z^2\overline{c}_Z^2}\,(S+U) \equiv \frac{\Pi_{WW}^{\text{new}}(m_W^2) - \Pi_{WW}^{\text{new}}(0)}{m_W^2} - \frac{\overline{c}_W}{\overline{s}_W}\frac{\Pi_{Z\gamma}^{\text{new}}(m_W^2)}{m_W^2} - \frac{\Pi_{\gamma\gamma}^{\text{new}}(m_W^2)}{m_W^2}\,, \tag{5.3}$$

where $\overline{s}_W \equiv \sin\theta_W(m_Z)$, $\overline{c}_W \equiv \cos\theta_W(m_Z)$, and $\overline{\alpha} \equiv \overline{g}^2\overline{s}_Z^2/(4\pi)$ are defined in the $\overline{\text{MS}}$ scheme evaluated at m_Z. The $\Pi_{V_aV_b}^{\text{new}}$ are the new physics contributions to the one-loop V_a—V_b vacuum polarization functions. New physics contributions are defined as those that enter relative to the Standard Model with a particular choice of the Standard Model Higgs mass (denoted in what follows by m_ϕ). In ref. [19], the value of $m_\phi = 117$ GeV is chosen.

In the linear approximation [8], which is a good approximation if the energy scale new physics that contributes to the oblique parameters is significantly larger than m_Z, we may approximate:

$$\Pi_{ij}^{\text{new}}(q^2) \simeq A_{ij}(0) + q^2 F_{ij}(q^2)\,. \tag{5.4}$$

Electromagnetic gauge invariance implies that:[26]

$$A_{\gamma\gamma}(0) = A_{Z\gamma}(0) = 0\,. \tag{5.5}$$

In the linear approximation, the oblique parameters take the following form [25]

$$\alpha T \equiv \frac{A_{WW}(0)}{m_W^2} - \frac{A_{ZZ}(0)}{m_Z^2} \tag{5.6}$$

$$\frac{g^2}{16\pi c_W^2}S \equiv F_{ZZ}(m_Z^2) - F_{\gamma\gamma}(m_Z^2) - \left(\frac{c_W^2 - s_W^2}{s_W c_W}\right)F_{Z\gamma}(m_Z^2) \tag{5.7}$$

$$\frac{g^2}{16\pi}(S+U) \equiv F_{WW}(m_W^2) - F_{\gamma\gamma}(m_W^2) - \frac{c_W}{s_W}F_{Z\gamma}(m_W^2)\,, \tag{5.8}$$

where we have dropped the bars for ease of notation.

The S, T and U parameters are defined relative to the Standard Model, so that $S = T = U = 0$ corresponds to the Standard Model with a particular "reference" choice of the Higgs mass m_ϕ. The 2HDM yields new contributions to S, T and U that in general shift their values away from zero. To compute the 2HDM contributions to S, T and U, we evaluate the relevant one-loop gauge boson polarization functions in which the Higgs bosons appear as intermediate states, and then subtract out the corresponding contributions due to the Standard Model Higgs boson of mass m_ϕ. In our computations, we initially leave m_ϕ as a free parameter.

5.1. 2HDM contributions to S, T and U

The derivations of S, T and U are provided in Appendix D. The 2HDM contributions to S are given by:

$$\begin{aligned}
S = \frac{1}{\pi m_Z^2}\Bigg\{ &\sum_{k=1}^{3} q_{k1}^2\Big[\mathcal{B}_{22}(m_Z^2; m_Z^2, m_k^2) - m_Z^2\mathcal{B}_0(m_Z^2; m_Z^2, m_k^2)\Big]\\
&+q_{11}^2\mathcal{B}_{22}(m_Z^2; m_2^2, m_3^2) + q_{21}^2\mathcal{B}_{22}(m_Z^2; m_1^2, m_3^2) + q_{31}^2\mathcal{B}_{22}(m_Z^2; m_1^2, m_2^2)\\
&-\mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_{H^\pm}^2) - \mathcal{B}_{22}(m_Z^2; m_Z^2, m_\phi^2) + m_Z^2\mathcal{B}_0(m_Z^2; m_Z^2, m_\phi^2)\Bigg\}\,,
\end{aligned} \tag{5.9}$$

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[25] In the definition of U, we differ slightly from that of ref. [19] by evaluating $\Pi_{Z\gamma}^{\text{new}}$ and $\Pi_{\gamma\gamma}^{\text{new}}$ at m_W^2 (instead of m_Z^2). This choice was advocated in ref. [24].

[26] Although $\Pi_{Z\gamma}(0) \neq 0$ (when all Standard Model contributions are included), the new physics contributions to $\Pi_{Z\gamma}(0)$ considered in this paper can be shown to vanish as a consequence of electromagnetic gauge invariance.

where

$$\mathcal{B}_{22}(q^2; m_1^2, m_2^2) \equiv B_{22}(q^2; m_1^2, m_2^2) - B_{22}(0; m_1^2, m_2^2), \tag{5.10}$$

$$\mathcal{B}_0(q^2; m_1^2, m_2^2) \equiv B_0(q^2; m_1^2, m_2^2) - B_0(0; m_1^2, m_2^2), \tag{5.11}$$

and the m_k are the masses of the neutral Higgs h_k ($k = 1, 2, 3$). The functions B_{22} and B_0 appearing in eqs. (5.10) and (5.11), defined in ref. [26], arise in the evaluation of the two-point loop integrals. They can be evaluated in dimensional regularization using the following formulae of ref. [25]:

$$B_{22}(q^2; m_1^2, m_2^2) = \tfrac{1}{4}(\Delta + 1)[m_1^2 + m_2^2 - \tfrac{1}{3}q^2] - \tfrac{1}{2}\int_0^1 dx X \ln(X - i\epsilon), \tag{5.12}$$

$$B_0(q^2; m_1^2, m_2^2) = \Delta - \int_0^1 dx \ln(X - i\epsilon), \tag{5.13}$$

where

$$X \equiv m_1^2 x + m_2^2(1 - x) - q^2 x(1 - x), \qquad \Delta \equiv \frac{2}{4 - d} + \ln 4\pi - \gamma, \tag{5.14}$$

in d space-time dimensions. Note that

$$B_{22}(q^2; m_1^2, m_2^2) = B_{22}(q^2; m_2^2, m_1^2), \qquad B_0(q^2; m_1^2, m_2^2) = B_0(q^2; m_2^2, m_1^2). \tag{5.15}$$

The 2HDM contributions to T and $U + S$ are given by:

$$\begin{aligned}
T = \frac{1}{16\pi m_W^2 s_W^2} \Bigg\{ &\sum_{k=1}^{3} |q_{k2}|^2 \mathcal{F}(m_{H^\pm}^2, m_k^2) - q_{11}^2 \mathcal{F}(m_2^2, m_3^2) - q_{21}^2 \mathcal{F}(m_1^2, m_3^2) - q_{31}^2 \mathcal{F}(m_1^2, m_2^2) \\
&+ \sum_{k=1}^{3} q_{k1}^2 \left[\mathcal{F}(m_W^2, m_k^2) - \mathcal{F}(m_Z^2, m_k^2) - 4m_W^2 B_0(0; m_W^2, m_k^2) + 4m_Z^2 B_0(0; m_Z^2, m_k^2) \right] \\
&+ \mathcal{F}(m_Z^2, m_\phi^2) - \mathcal{F}(m_W^2, m_\phi^2) + 4m_W^2 B_0(0; m_W^2, m_\phi^2) - 4m_Z^2 B_0(0; m_Z^2, m_\phi^2) \Bigg\},
\end{aligned} \tag{5.16}$$

$$\begin{aligned}
S + U = \frac{1}{\pi m_W^2} \Bigg\{ &-\sum_{k=1}^{3} q_{k1}^2 m_W^2 \mathcal{B}_0(m_W^2; m_W^2, m_k^2) + m_W^2 \mathcal{B}_0(m_W^2; m_W^2, m_\phi^2) - \mathcal{B}_{22}(m_W^2; m_W^2, m_\phi^2) \\
&+ \sum_{k=1}^{3} \left[q_{k1}^2 \mathcal{B}_{22}(m_W^2; m_W^2, m_k^2) + |q_{k2}|^2 \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_k^2) \right] - 2\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) \Bigg\},
\end{aligned} \tag{5.17}$$

where the function $\mathcal{F}$ is defined by

$$\mathcal{F}(m_1^2, m_2^2) \equiv \tfrac{1}{2}(m_1^2 + m_2^2) - \frac{m_1^2 m_2^2}{m_1^2 - m_2^2} \ln\left(\frac{m_1^2}{m_2^2}\right). \tag{5.18}$$

Note that

$$\mathcal{F}(m_1^2, m_2^2) = \mathcal{F}(m_2^2, m_1^2), \qquad \mathcal{F}(m^2, m^2) = 0. \tag{5.19}$$

One can simplify the expression for T by making use of the identity:

$$m_1^2 B_0(0; m_1^2, m_3^2) - m_2^2 B_0(0; m_2^2, m_3^2) = \mathcal{F}(m_1^2, m_3^2) - \mathcal{F}(m_2^2, m_3^2) + A_0(m_1^2) - A_0(m_2^2) - \tfrac{1}{2}(m_1^2 - m_2^2), \tag{5.20}$$

where

$$A_0(m^2) \equiv m^2(\Delta + 1 - \ln m^2). \tag{5.21}$$

	TABLE X:

Case I: $s_{13} = 0$. In a real basis, $e^{-i\theta_{23}} = \text{sgn } Z_6 \equiv \varepsilon_6$. The neutral Higgs fields are $h_1 = h^0$, $h_2 = -\varepsilon_6 H^0$ and $h_3 = \varepsilon_6 A^0$. The angular factors are $c_{12} = \sin(\beta - \alpha)$ and $s_{12} = -\varepsilon_6 \cos(\beta - \alpha)$.

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

TABLE XI:
Case IIa: $s_{12} = 0$. In a real basis, $e^{-i\theta_{23}} = i\,\text{sgn } Z_6 \equiv i\varepsilon_6$. The neutral Higgs fields are $h_1 = h^0$, $h_2 = \varepsilon_6 A^0$ and $h_3 = \varepsilon_6 H^0$. The angular factors are $c_{13} = \sin(\beta - \alpha)$ and $s_{13} = \varepsilon_6 \cos(\beta - \alpha)$.

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

TABLE XII:
Case IIb: $c_{12} = 0$. In a real basis, $e^{-i\theta_{23}} = i\,\text{sgn } Z_6 \equiv i\varepsilon_6$. The neutral Higgs fields are $h_1 = \varepsilon_6 A^0$, $h_2 = -h^0$ and $h_3 = \varepsilon_6 H^0$. The angular factors are $c_{13} = \sin(\beta - \alpha)$ and $s_{13} = \varepsilon_6 \cos(\beta - \alpha)$.

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

Applying the identity of eq. (5.20) in the expression for T then yields:

$$T = \frac{1}{16\pi m_W^2 s_W^2} \left\{ \sum_{k=1}^{3} |q_{k2}|^2 \mathcal{F}(m_{H^\pm}^2, m_k^2) - q_{11}^2 \mathcal{F}(m_2^2, m_3^2) - q_{21}^2 \mathcal{F}(m_1^2, m_3^2) - q_{31}^2 \mathcal{F}(m_1^2, m_2^2) \right.$$
$$\left. + 3\sum_{k=1}^{3} q_{k1}^2 \left[\mathcal{F}(m_Z^2, m_k^2) - \mathcal{F}(m_W^2, m_k^2) \right] - 3\left[\mathcal{F}(m_Z^2, m_\phi^2) - \mathcal{F}(m_W^2, m_\phi^2) \right] \right\}, \tag{5.22}$$

which reproduces the result first obtained in ref. [7]. In particular, note that terms in eq. (5.20) of the form $A_0(m_1^2) - A_0(m_2^2) - \frac{1}{2}(m_1^2 - m_2^2)$ are independent of m_3^2 and hence cancel out exactly in eq. (5.22).

Using eqs. (5.9) and (5.17), we can isolate the U-parameter,

$$U = \mathcal{G}(m_W^2) - \mathcal{G}(m_Z^2) + \frac{1}{\pi m_W^2} \left\{ \sum_{k=1}^{3} [|q_{k2}|^2 \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_k^2) - 2\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) \right\}$$
$$- \frac{1}{\pi m_Z} \left\{ q_{11}^2 \mathcal{B}_{22}(m_Z^2; m_2^2, m_3^2) + q_{21}^2 \mathcal{B}_{22}(m_Z^2; m_1^2, m_3^2) + q_{31}^2 \mathcal{B}_{22}(m_Z^2; m_1^2, m_2^2) - \mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_{H^\pm}^2) \right\}, \tag{5.23}$$

where

$$\mathcal{G}(m_V^2) \equiv \frac{1}{\pi m_V^2} \left\{ \sum_{k=1}^{3} q_{k1}^2 \left[\mathcal{B}_{22}(m_V^2; m_V^2, m_k^2) - m_V^2 \mathcal{B}_0(m_V^2; m_V^2, m_k^2) \right] - \mathcal{B}_{22}(m_V^2; m_V^2, m_\phi^2) + m_V^2 \mathcal{B}_0(m_V^2; m_V^2, m_\phi^2) \right\}. \tag{5.24}$$

5.2. S, T, and U in the CP-conserving limit

To obtain S, T and U in the CP-conserving limit, we must identify the values of q_{k1} and q_{k2} and the corresponding neutral Higgs masses m_k in the CP-conserving limit. For example, in ref. [2], the values of the $q_{k\ell}$ and m_k were obtained for Cases I, IIa and IIb defined in Section 3.1. For the reader's convenience, we reproduce those results here in Tables X–XII. These three cases correspond to three different mass orderings of the neutral Higgs bosons (by assumption, we assume here that $m_{h_1} < m_{h_2} < m_{h_3}$).

In the CP-conserving limit, it is traditional to employ the factors $\cos(\beta - \alpha)$ and $\sin(\beta - \alpha)$, where α is the mixing angle obtained from diagonalizing the 2×2 CP-even Higgs squared-mass matrix in a generic real basis [12]. These angle factors are related to the $q_{k\ell}$ as indicated in the captions to Tables X–XII. The results for S, T and U do not depend on which Case is employed to compute the $q_{k\ell}$, since the different cases simply correspond to different mass-orderings of the neutral Higgs bosons. Plugging in the values of the $q_{k\ell}$ parameters from any of the Cases exhibited in Tables X–XII into eqs. (5.9)–(5.17), and choosing the reference Higgs mass $m_\phi = m_{h^0}$ (where h^0 is the

lightest CP-even neutral Higgs boson), we obtain:

$$S = \frac{1}{\pi m_Z^2}\left\{-\mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_{H^\pm}^2) + \sin^2(\beta-\alpha)\mathcal{B}_{22}(m_Z^2; m_{H^0}^2, m_{A^0}^2)\right.$$

$$+ \cos^2(\beta-\alpha)\left[\mathcal{B}_{22}(m_Z^2; m_{h^0}^2, m_{A^0}^2) + \mathcal{B}_{22}(m_Z^2; m_Z^2, m_{H^0}^2) - \mathcal{B}_{22}(m_Z^2; m_Z^2, m_{h^0}^2)\right.$$

$$\left.\left. -m_Z^2\mathcal{B}_0(m_Z^2; m_Z^2, m_{H^0}^2) + m_Z^2\mathcal{B}_0(m_Z^2; m_Z^2, m_{h^0}^2)\right]\right\}, \tag{5.25}$$

$$T = \frac{1}{16\pi s_W^2 m_W^2}\left\{\mathcal{F}(m_{H^\pm}^2, m_{A^0}^2) + \sin^2(\beta-\alpha)\left[\mathcal{F}(m_{H^\pm}^2, m_{H^0}^2) - \mathcal{F}(m_{A^0}^2, m_{H^0}^2)\right]\right.$$

$$+ \cos^2(\beta-\alpha)\left[\mathcal{F}(m_{H^\pm}^2, m_{h^0}^2) - \mathcal{F}(m_{A^0}^2, m_{h^0}^2) + \mathcal{F}(m_W^2, m_{H^0}^2) - \mathcal{F}(m_W^2, m_{h^0}^2)\right.$$

$$-\mathcal{F}(m_Z^2, m_{H^0}^2) + \mathcal{F}(m_Z^2, m_{h^0}^2) + 4m_Z^2 B_0(0; m_Z^2, m_{H^0}^2) - 4m_Z^2 B_0(0; m_Z^2, m_{h^0}^2)$$

$$\left.\left. -4m_W^2 B_0(0; m_W^2, m_{H^0}^2) + 4m_W^2 B_0(0; m_W^2, m_{h^0}^2)\right]\right\}, \tag{5.26}$$

$$S + U = \frac{1}{\pi m_W^2}\left\{\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{A^0}^2) - 2\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) + \sin^2(\beta-\alpha)\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^0}^2)\right.$$

$$+ \cos^2(\beta-\alpha)\left[\mathcal{B}_{22}(m_W^2; m_{h^0}^2, m_{H^\pm}^2) + \mathcal{B}_{22}(m_W^2; m_W^2, m_{H^0}^2) - \mathcal{B}_{22}(m_W^2; m_W^2, m_{h^0}^2)\right.$$

$$\left.\left. +m_W^2\mathcal{B}_0(m_W^2; m_W^2, m_{H^0}^2) - m_W^2\mathcal{B}_0(m_W^2; m_W^2, m_{h^0}^2)\right]\right\}. \tag{5.27}$$

The above results agree with results previously obtained in refs. [25] and [27].[27]

5.3. T and U and the custodial limit

In the custodial symmetric limit, both the T and U-parameters must vanish [8]. Using eq. (5.22), we can verify this behavior. In the 2HDM, custodial symmetry-breaking arises from two sources. The first source is the gauged U(1)-hypercharge interactions that are always present. The second source is the custodial symmetry-breaking terms of the scalar potential. Let us look at both sources in turn.

We can formally restore custodial symmetry in the gauge sector by taking the limit of $g' \to 0$ (in which case, $m_Z = m_W$). If we set $m_W = m_Z$ in eq. (5.22), we see that the second line of this equation vanishes. That is, the second line of eq. (5.22) is a consequence of the gauged U(1)-hypercharge interactions. Formally, this term must be proportional to g'. Noting that

$$\frac{\alpha}{s_W^2 m_W^2} = \frac{g^2}{4\pi^2 m_W^2} = \frac{g'^2}{4\pi(m_Z^2 - m_W^2)}, \tag{5.28}$$

it follows that

$$\alpha T = \frac{3g'^2}{64\pi^2(m_Z^2 - m_W^2)}\left\{\sum_{k=1}^{3} q_{k1}^2\left[\mathcal{F}(m_Z^2, m_k^2) - \mathcal{F}(m_W^2, m_k^2)\right] - \mathcal{F}(m_Z^2, m_\phi^2) + \mathcal{F}(m_W^2, m_\phi^2)\right\}$$

$$+ \frac{g^2}{64\pi m_W^2}\left\{\sum_{k=1}^{3} |q_{k2}|^2\mathcal{F}(m_{H^\pm}^2, m_k^2) - q_{11}^2\mathcal{F}(m_2^2, m_3^2) - q_{21}^2\mathcal{F}(m_1^2, m_3^2) - q_{31}^2\mathcal{F}(m_1^2, m_2^2)\right\}. \tag{5.29}$$

In this form, one can explicitly identify the term in T proportional to g' as the piece that arises from the gauged U(1)-hypercharge interactions.[28]

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[27] In eq. (3.47) of ref. [25], there is a typographical error in the expression for T. The right bracket at the end of the third line of eq. (3.47) is misplaced and should appear at the end of the fifth line.

[28] Note that the expression in eq. (5.29) that multiplies g'^2 approaches a finite limit as $m_Z \to m_W$. Hence, the entire term does indeed vanish in the custodial symmetry limit as expected.

The term proportional to g in eq. (5.29) arises as a consequence of custodial symmetry breaking in the scalar potential. Thus, we should verify that this term vanishes in the limit of a custodial symmetric scalar potential. In this limit, CP is conserved, so we may use the results of Table X–XII to evaluate eq. (5.29) [any one of the three Cases can be used as noted in the previous subsection]. For convenience, we again choose $m_\phi = m_{h^0}$, in which case,

$$\alpha T = \frac{3g'^2 \cos^2(\beta - \alpha)}{64\pi^2(m_Z^2 - m_W^2)} \left\{ \mathcal{F}(m_Z^2, m_{H^0}^2) - \mathcal{F}(m_W^2, m_{H^0}^2) - \mathcal{F}(m_Z^2, m_{h^0}^2) + \mathcal{F}(m_W^2, m_{m_h^0}) \right\}$$

$$+ \frac{g^2}{64\pi m_W^2} \left\{ \mathcal{F}(m_{H^\pm}^2, m_{A^0}^2) + \sin^2(\beta - \alpha) \left[\mathcal{F}(m_{H^\pm}^2, m_{H^0}^2) - \mathcal{F}(m_{A^0}^2, m_{H^0}^2) \right] \right.$$

$$\left. + \cos^2(\beta - \alpha) \left[\mathcal{F}(m_{H^\pm}^2, m_{h^0}^2) - \mathcal{F}(m_{A^0}^2, m_{h^0}^2) \right] \right\}. \tag{5.30}$$

For a custodial symmetric scalar potential, the term proportional to g^2 in eq. (5.30) must vanish, i.e.

$$\mathcal{F}(m_{H^\pm}^2, m_{A^0}^2) + \sin^2(\beta - \alpha) \left[\mathcal{F}(m_{H^\pm}^2, m_{H^0}^2) - \mathcal{F}(m_{A^0}^2, m_{H^0}^2) \right] + \cos^2(\beta - \alpha) \left[\mathcal{F}(m_{H^\pm}^2, m_{h^0}^2) - \mathcal{F}(m_{A^0}^2, m_{h^0}^2) \right] = 0. \tag{5.31}$$

In Section 4.1.3, we demonstrated that for a custodial symmetric scalar potential, $m_{H^\pm}^2 = m_{A^0}^2$ [cf. eq. (4.49)], in nearly all cases. Indeed, for $\sin(\beta - \alpha) \cos(\beta - \alpha) \neq 0$, the only solution to eq. (5.31) is $m_{H^\pm}^2 = m_{A^0}^2$. However, we identified the special case of $Z_6 = Z_7 = 0$ in which the custodial symmetric scalar potential could also yield $m_{H^\pm}^2 = m_{h^0}^2$ or $m_{H^\pm}^2 = m_{H^0}^2$ [cf. eq. (4.51)]. For example, by comparing Table X with Tables VII and VIII, we see that the special case of $Z_6 = Z_7 = 0$ corresponds to $\cos(\beta - \alpha) = 0$ and $\sin(\beta - \alpha) = 0$, respectively. In these two cases, eq. (5.31) reduces to the following two equations:

$$\mathcal{F}(m_{H^\pm}^2, m_{A^0}^2) + \mathcal{F}(m_{H^\pm}^2, m_{H^0}^2) - \mathcal{F}(m_{A^0}^2, m_{H^0}^2) = 0, \qquad \text{if } \cos(\beta - \alpha) = 0, \tag{5.32}$$

$$\mathcal{F}(m_{H^\pm}^2, m_{A^0}^2) + \mathcal{F}(m_{H^\pm}^2, m_{h^0}^2) - \mathcal{F}(m_{A^0}^2, m_{h^0}^2) = 0 \qquad \text{if } \sin(\beta - \alpha) = 0. \tag{5.33}$$

Of course, $m_{H^\pm}^2 = m_{A^0}^2$ remains as a possible solution to both of the above equations. But, for each equation above, a second solution exists, namely $m_{H^\pm}^2 = m_{H^0}^2$ for eq. (5.32) and $m_{H^\pm}^2 = m_{h^0}^2$ for eq. (5.33). Thus, we confirm that in the case of $Z_6 = Z_7 = 0$, the custodial symmetric mass relations identified in eq. (4.51) are consistent with the vanishing of the T parameter (in the limit of $g' = 0$ and $m_W = m_Z$).

So far, we have focused on the contributions of the bosonic sector of the 2HDM to the T parameter. In addition, there are also fermion loop contributions since the Higgs–fermion Yukawa interactions can also violate the custodial symmetry. However, at one-loop, the only custodial-violating contribution to the T-parameter arises due to the non-degeneracy of the up and down fermion mass matrices. But, this effect also is present in the Standard Model with one Higgs doublet, as first noted in ref. [23]. New custodial symmetry breaking effects in the Higgs–fermion Yukawa interactions that are present due to the second Higgs doublet must involve ρ^Q. Since the dependence of the gauge boson polarization functions on ρ^Q only enters at two loops in the perturbative expansion, we shall not include them in the present analysis. It would be an interesting exercise to verify that the corresponding two-loop contributions to the T parameter vanish exactly in the custodial symmetric limit specified in eq. (4.67).

The analysis of the U-parameter is similar. Using eqs. (5.23) and (5.24), we see that when $m_W = m_Z$, the general expression for U reduces to:

$$U = \frac{1}{\pi m_W^2} \left\{ \sum_{k=1}^3 [|q_{k2}|^2 \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_k^2) - q_{11}^2 \mathcal{B}_{22}(m_W^2; m_2^2, m_3^2) - q_{21}^2 \mathcal{B}_{22}(m_W^2; m_1^2, m_3^2) \right.$$

$$\left. - q_{31}^2 \mathcal{B}_{22}(m_W^2; m_1^2, m_2^2) - \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) \right\}. \tag{5.34}$$

In the CP-conserving limit (with $m_W = m_Z$),

$$U = \frac{1}{\pi m_W^2} \left\{ \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_A^2) - \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) \right.$$

$$+ \sin^2(\beta - \alpha) \left[\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^0}^2) - \mathcal{B}_{22}(m_W^2; m_{H^0}^2, m_{A^0}^2) \right]$$

$$\left. + \cos^2(\beta - \alpha) \left[\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{h^0}^2) - \mathcal{B}_{22}(m_W^2; m_{h^0}^2, m_{A^0}^2) \right] \right\}. \tag{5.35}$$

If $\sin(\beta - \alpha)\cos(\beta - \alpha) \neq 0$, then $U = 0$ if and only if $m_{H^\pm}^2 = m_{A^0}^2$. In the special case of $Z_6 = Z_7 = 0$, it follows that either $\sin(\beta - \alpha) = 0$ or $\cos(\beta - \alpha) = 0$, in which case $U = 0$ when

$$\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_A^2) - \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) + \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^0}^2) - \mathcal{B}_{22}(m_W^2; m_{H^0}^2, m_{A^0}^2) = 0\,,$$
$$\text{if } \cos(\beta - \alpha) = 0\,, \tag{5.36}$$

$$\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_A^2) - \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) + \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{h^0}^2) - \mathcal{B}_{22}(m_W^2; m_{h^0}^2, m_{A^0}^2) = 0\,,$$
$$\text{if } \sin(\beta - \alpha) = 0\,. \tag{5.37}$$

Of course, $m_{H^\pm}^2 = m_{A^0}^2$ remains as a possible solution to both of the above equations. But, for each equation above, a second solution exists, namely $m_{H^\pm}^2 = m_{H^0}^2$ for eq. (5.37) and $m_{H^\pm}^2 = m_{h^0}^2$ for eq. (5.37). Thus, we confirm that in the case of $Z_6 = Z_7 = 0$, the custodial symmetric mass relations identified in eq. (4.51) are consistent with the vanishing of the U parameter.

5.4. S, T and U in the decoupling limit

In the decoupling limit of the 2HDM [28], one neutral Higgs boson, conventionally denoted by h_1, is kept light, with mass $m_1 \lesssim \mathcal{O}(m_Z)$, and the other neutral Higgs bosons h_2 and h_3 and the charged Higgs boson $H^\pm$ have masses of order $\Lambda \gg m_Z$. In Appendix E, the Higgs masses and invariant mixing angles are evaluated in the decoupling limit. The resulting masses are given in eqs. (E.21)–(E.24) and the invariant mixing angles are given in eq. (E.28). The explicit forms for the q_{ki} given in Table I are given by

$$q_{11}^2 \simeq |q_{22}|^2 \simeq |q_{32}|^2 \simeq 1 - \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right)\,, \qquad q_{21}^2 \simeq q_{31}^2 \simeq |q_{12}|^2 \simeq \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right)\,. \tag{5.38}$$

We now turn to the computation of the oblique parameters in the decoupling limit. As a first step, we eliminate q_{11} in favor of q_{21} and q_{31} using the identity,

$$\sum_{i=1}^{3} q_{k1}^2 = 1\,. \tag{5.39}$$

It is also convenient to set the reference Higgs mass $m_\phi = m_1$. Then, one can write the general expression for S as follows:

$$\begin{aligned}
S = \frac{1}{\pi m_Z^2}\Big\{ &\mathcal{B}_{22}(m_Z^2; m_2^2, m_3^2) - \mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_{H^\pm}^2) \\
&+ q_{21}^2\left[\mathcal{B}_{22}(m_Z^2; m_Z^2, m_2^2) + \mathcal{B}_{22}(m_Z^2; m_1^2, m_3^2) - m_Z^2 \mathcal{B}_0(m_Z^2; m_Z^2, m_2^2)\right] \\
&+ q_{31}^2\left[\mathcal{B}_{22}(m_Z^2; m_Z^2, m_3^2) + \mathcal{B}_{22}(m_Z^2; m_1^2, m_2^2) - m_Z^2 \mathcal{B}_0(m_Z^2; m_Z^2, m_3^2)\right] \\
&- (q_{21}^2 + q_{31}^2)\left[\mathcal{B}_{22}(m_Z^2; m_2^2, m_3^2) + \mathcal{B}_{22}(m_Z^2; m_Z^2, m_1^2) - m_Z^2 \mathcal{B}_0(m_Z^2; m_Z^2, m_1^2)\right]\Big\}\,.
\end{aligned} \tag{5.40}$$

Employing the decoupling limit conditions of eq. (5.38),

$$S = \frac{1}{\pi m_Z^2}\left[\mathcal{B}_{22}(m_Z^2; m_2^2, m_3^2) - \mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_{H^\pm}^2) + \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right)\right]\,. \tag{5.41}$$

Using eqs. (E.29)–(E.31) and noting the expansion,

$$\mathcal{B}_{22}(m_Z^2; \Lambda^2 + av^2, \Lambda^2 + bv^2) = -\tfrac{1}{12}m_Z^2\left[\Delta - \ln\Lambda^2 - \frac{(a+b)v^2}{2\Lambda^2} + \frac{m_Z^2}{10\Lambda^2} + \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right)\right]\,, \tag{5.42}$$

it then follows that:

$$S \simeq \frac{m_2^2 + m_3^2 - 2m_{H^\pm}^2}{24\pi m_3^2} = \frac{Z_4 v^2}{24\pi m_3^2}\,, \tag{5.43}$$

where terms of $\mathcal{O}(v^2/\Lambda^4)$ have been neglected.

One can evaluate T in a similar manner. Setting $m_\phi = m_1$ in eq. (5.16), and employing the decoupling limit conditions of eq. (5.38), we obtain:

$$T = \frac{1}{16\pi s_W^2 m_W^2} \left[\mathcal{F}(m_{H^\pm}^2, m_2^2) + \mathcal{F}(m_{H^\pm}^2, m_3^2) - \mathcal{F}(m_2^2, m_3^2) + \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right) \right] . \tag{5.44}$$

Using eqs. (E.29)–(E.31) and noting the expansion,

$$\mathcal{F}(\Lambda^2 + av^2, \Lambda^2 + bv^2) \simeq \tfrac{1}{6}v^2 \left[\frac{(a-b)^2}{\Lambda^2} + \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right) \right] , \tag{5.45}$$

it then follows that:

$$T \simeq \frac{(m_{H^\pm}^2 - m_3^2)(m_{H^\pm}^2 - m_2^2)}{48\pi s_W^2 m_W^2 m_3^2} = \frac{(Z_4^2 - |Z_5|^2)v^2}{48\pi e^2 m_3^2} , \tag{5.46}$$

after using $e = gs_W = 2s_W m_W/v$. In the custodial limit, $H^\pm$ is degenerate in mass with either h_2 or h_3,[29] in which case T must vanish. Indeed, eq. (5.46) satisfies this requirement. This result is not surprising since to leading order in the decoupling limit, we may set $\cos(\beta - \alpha) = 0$ in which case eq. (5.32) applies.

As a check of the above computations, one can use eqs. (5.43) and (5.46) to calculate the contributions of the Higgs sector of the minimal supersymmetric Standard Model (MSSM) to S and T in the decoupling limit. The quartic couplings of the MSSM Higgs potential, defined in a supersymmetric basis [29], satisfy:

$$\lambda_1 = \lambda_2 = \tfrac{1}{4}(g^2 + g'^2), \qquad \lambda_3 = \tfrac{1}{4}(g^2 - g'^2), \qquad \lambda_4 = -\tfrac{1}{2}g^2, \qquad \lambda_5 = \lambda_6 = \lambda_7 = 0, \tag{5.47}$$

where the λ_i are defined in eq. (4.2). In the supersymmetric basis, the ratio of vacuum expectation values is $\tan\beta \equiv v_2/v_1$. Since the MSSM Higgs sector is CP-conserving, one can transform to the *real* Higgs basis, which yields:

$$Z_1 = Z_2 = \tfrac{1}{4}(g^2 + g'^2)\cos^2 2\beta, \qquad Z_5 = \tfrac{1}{4}(g^2 + g'^2)\sin^2 2\beta, \qquad Z_7 = -Z_6 = \tfrac{1}{4}(g^2 + g'^2)\sin 2\beta \cos 2\beta, \tag{5.48}$$

$$Z_3 = \tfrac{1}{4}\left[(g^2 + g'^2)\sin^2 2\beta + g^2 - g'^2\right] , \qquad Z_4 = \tfrac{1}{4}\left[(g^2 + g'^2)\sin^2 2\beta - 2g^2\right] . \tag{5.49}$$

Note that $Z_5 > 0$ which means that $\varepsilon_{56} = \varepsilon_{57} = +1$. Using eqs. (2.22) and (3.17) yields the exact (tree-level) mass relation,

$$m_{H^\pm}^2 = m_{A^0}^2 + m_W^2 . \tag{5.50}$$

Moreover, in the decoupling limit, eq. (E.30) yields $m_{H^0}^2 = m_{A^0}^2 + Z_5 v^2 + \mathcal{O}(v^2/m_{A^0}^2)$, which can be rewritten using eq. (5.48),

$$m_{H^0}^2 = m_{A^0}^2 + m_Z^2 \sin^2 2\beta + \mathcal{O}(v^2/m_{A^0}^2). \tag{5.51}$$

Substituting eqs. (5.48) and (5.49) [or equivalently, eqs. (5.50) and (5.51)] into eqs. (5.43) and (5.46) yields

$$S_{\mathrm{MSSM}} \simeq \frac{m_Z^2 \sin^2 2\beta - 2m_W^2}{24\pi m_{A^0}^2},$$

$$T_{\mathrm{MSSM}} \simeq \frac{m_W^2 - m_Z^2 \sin^2 2\beta}{48\pi s_W^2 m_{A^0}^2}, \tag{5.52}$$

which reproduce the results previously obtained in ref. [25].

Finally, we examine U in the decoupling limit. Setting $m_\phi = m_1$ in eq. (5.17) and employing the decoupling limit conditions of eq. (5.38), we obtain:

$$S + U = \frac{1}{\pi m_W^2} \left[\mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_2^2) + \mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_3^2) - 2\mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_{H^\pm}^2) + \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right) \right] . \tag{5.53}$$

---

[29] In general $H^\pm$ is degenerate in mass with A^0 whose identity (either h_2 or h_3) is determined from eqs. (E.32) and (E.33). If $Z_6 = Z_7 = 0$, $H^\pm$ may instead be degenerate in mass with H^0 in the custodial limit as noted in eq. (4.51). Of course, in the decoupling limit $H^\pm$ can never be degenerate in mass with h^0 since $m_{h^0} \ll m_{H^\pm}$.

Using eqs. (E.22) and (E.23) and eq. (5.42), we obtain:

$$S + U \simeq \frac{m_2^2 + m_3^2 - 2m_{H^\pm}^2}{24\pi c_W^2 m_3^2} = \frac{Z_4 v^2}{24\pi c_W^2 m_3^2} = \frac{S}{c_W^2} \,. \tag{5.54}$$

Finally, we use eq. (5.43) to isolate U:

$$U \simeq S \tan^2 \theta_W \,. \tag{5.55}$$

In the custodial limit where $g' = 0$, it follows that $\tan \theta_W = 0$, in which case $U = 0$. Remarkably, we find that $U = 0$ in this limit independently of the values of the neutral Higgs masses. Thus, custodial symmetry breaking effects arising from the scalar potential do *not* generate a non-zero value for U at $\mathcal{O}(v^2/\Lambda^2)$ in the approach to the decoupling limit. However, eqs. (5.35)–(5.37) imply that a non-zero value for U would be generated at order $\mathcal{O}(v^4/\Lambda^4)$. This observation suggests that $U \ll T$ over a significant range of the 2HDM parameter space, a fact that can be verified numerically.

6. NUMERICAL ANALYSIS

The parameters S, T and U obtained from an analysis of precision electroweak data are found to be [19]:

$$
\begin{aligned}
S &= 0.01 \pm 0.10, \\
T &= 0.03 \pm 0.11, \\
U &= 0.06 \pm 0.10,
\end{aligned}
\tag{6.1}
$$

relative to the Standard Model, with a reference Higgs mass of $m_\phi = 117$ GeV. Similar results have been obtained by the GFITTER collaboration [20]. Alternatively, if one assumes that $U = 0$ (typically, one expects $U \ll S$ in many models of new physics beyond the Standard Model), then the corresponding analysis of S and T yields [19]:

$$S = 0.03 \pm 0.09, \qquad T = 0.07 \pm 0.08. \tag{6.2}$$

These limits indicate that new physics contributions to the oblique parameters are tightly constrained. In particular, if one assumes that the new physics contributions to S, T and U arise solely from the 2HDM sector, then eqs. (6.1) and (6.2) would constrain the parameters of the 2HDM scalar potential. Such studies have appeared in the literature in a less general framework. For example, in ref. [30], $\rho \equiv \alpha T$ was used to constrain a modified version of the 2HDM in which certain scalar couplings were set equal to zero, and $\tan \beta$ was assumed to be a physical observable. In our approach, only basis-independent quantities are employed. A full numerical study of the constraints of precision electroweak data on the general 2HDM contributions to the oblique parameters will be presented elsewhere (for a preliminary study, see ref. [31]). In this section, we shall outline our analysis methods and describe some of the key results and features of our study.

The parameters of the 2HDM that are constrained by S, T, and U can be taken to be Z_1, Z_3, $Z_3 + Z_4$, $Z_5 \, e^{-2i\theta_{23}}$, $Z_6 \, e^{-i\theta_{23}}$ and Y_2, since these 6 quantities determine the physical Higgs masses [cf. eqs. (2.17) and (2.22)] and the invariant quantities $q_{k\ell}$ [specified in Table I]. We impose one theoretical constraint by demanding that the $|Z_i|$ do not exceed upper bounds corresponding to the requirement that all bosonic scattering amplitudes satisfy tree-level unitarity (the relevant upper bounds are derived in Appendix F). In order to compare with the determination of of S, T and U in ref. [19], we fix the reference Higgs mass at $m_\phi = 117$ GeV. The procedure used here to study the effect of the 2HDM on the oblique parameters was to choose random values of the six parameters in the space allowed by the tree-level unitarity bounds. Then the Higgs masses and $q_{k\ell}$ are calculated numerically and inserted into eqs. (5.9)–(5.17) to obtain S, T, and U for each point in the parameter space.

In our first study, we imposed an additional requirement that the mass of the lightest neutral Higgs boson, m_1, fall within 10 GeV of the reference Higgs mass. It was found that the 2HDM consistently produces values of U within 0.02 of zero. Thus, in order to derive constraints on the 2HDM parameters, one can reliably set $U = 0$ and compare the computed S and T values of the 2HDM with the results given in eq. (6.2). Scanning the 2HDM parameter space and comparing with the allowed 2 σ contour ellipse in S–T plane produces the results shown in Fig. 1.

From the scatter plots shown in Fig. 1, it is evident that the values of S produced are all consistent with the experimental constraints of eq. (6.2). In contrast, there are many points that lie outside the allowed range for T. These points correspond to 2HDM parameters that significantly violate the custodial symmetry of the scalar potential. In particular, one must have a significant splitting between the masses of the $H^\pm$ and one of the heavy neutral Higgs bosons (identified in the generic CP-conserving 2HDM as A^0). This region of parameter space is very far away from
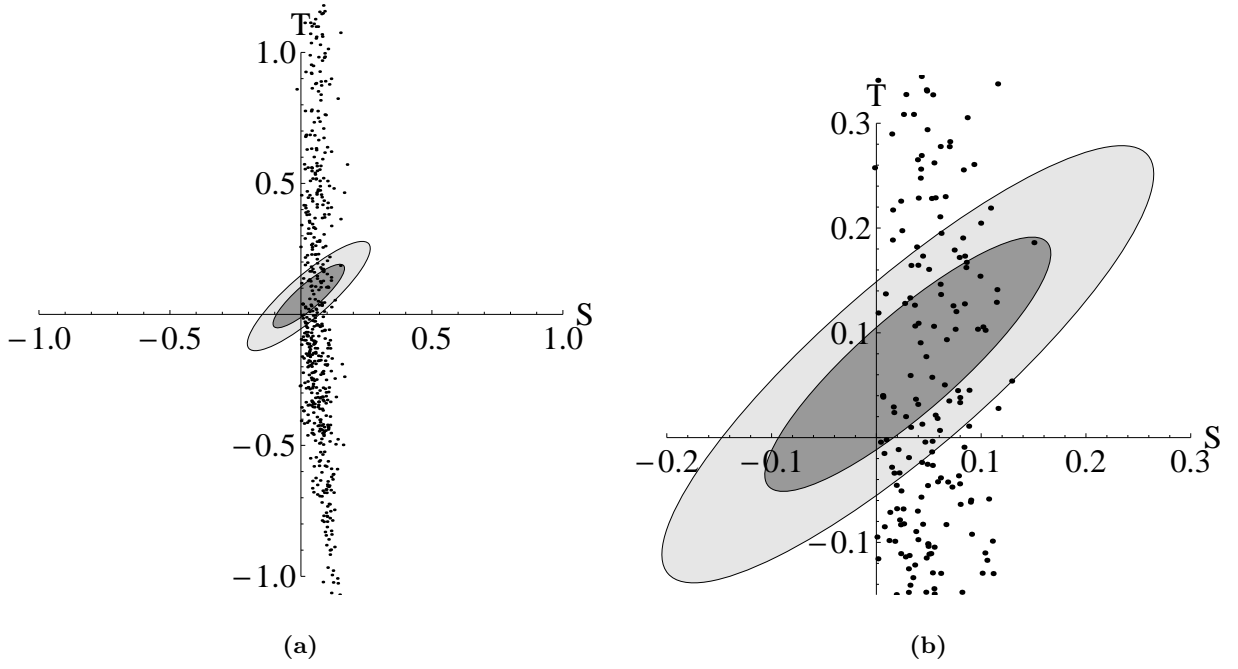
FIG. 1: Scatter plots for T as a function of S, with $m_1 = 117 \pm 10$ GeV. The ellipses, representing the 1 σ and 2 σ contours allowed by precision electroweak data, are based on ref. [19], with the parameter U fixed to zero. Plot (a) shows the expanded view in the S–T plane, and plot (b) shows a close-up view of the allowed region.

the decoupling region in which the 2HDM contributions to T are quite small. When T is large, the large values of the corresponding heavy Higgs masses are driven primarily by large values of the $Z_i v^2$ that compete with (and in some regions dominate) the contribution of Y_2. Even though the maximal values of the Z_i are constrained by tree-level unitarity, there is still a robust region of the 2HDM parameter space in which $|T|$ lies significantly outside of the interval allowed by eq. (6.2). It is also interesting to note that both positive and negative signs for T are allowed, with roughly equal probability over the 2HDM parameter space.

In the analysis above, we have fixed the value of the lightest neutral Higgs mass, m_1, to be close to 117 GeV. One can now investigate the consequence of relaxing this assumption. First, consider the decoupling limit of the 2HDM where $m_1 \ll m_2, m_3$. As m_1 increases (in a mass regime in which h_1 is still significantly lighter than h_2 and h_3), we should simply reproduce the known constraints of precision electroweak observables on the mass of m_1. As a concrete example, consider the following input parameters:

$$m_\phi = 117 \text{ GeV}, \quad Z_1 = 0.227, \quad Y_2 = (1 \text{ TeV})^2, \tag{6.3}$$

with all other invariant Z parameters equal to 0.01. The mass spectrum corresponding to these values is $m_1 = 117$ GeV, $m_2 = m_3 = m_{H^\pm} = 1$ TeV. As expected, in this limit one finds that $S \simeq T \simeq 0$. As Z_1 is increased from 0.227 to 0.505, m_1 increases from 117 GeV to 175 GeV, at which point T and S exceed the boundary of the 2 σ ellipse. In Fig. 2, the resulting S and T are shown as m_1 is varied from 117 GeV to 500 GeV.

If we depart significantly from the decoupling limit, then the custodial-symmetry breaking mass splitting between the $H^\pm$ and one of the heavy neutral Higgs states can contribute positively to T and offset the negative T values shown in Fig. 2. In this way, values of the lightest Higgs boson mass above 150 GeV may still be consistent with precision electroweak data. This possibility is illustrated by the following example. With m_ϕ fixed at 117 GeV, let us choose $Y_2 = (50 \text{ GeV})^2$ and $Z_3 = 5.2$. This produces $m_{H^\pm} = 400$ GeV. With $Z_1 = 4$, Z_4 is adjusted such that $m_1 = 350$ GeV, with all other Z parameters set equal to 0.01. One can then dial up Z_3 (keeping m_1 fixed at 350 GeV by simultaneously adjusting Z_4) until S and T lie within the 2 σ contour ellipse. For the above choice of Z_1, the allowed range for the charged Higgs mass is 443 GeV $< m_{H^\pm} <$ 489 GeV, as shown in column (a) of Fig. 3. We can repeat this exercise by fixing Z_1 at its tree-level unitarity limit. In this case the allowed range is 470 GeV $< m_{H^\pm} <$ 505 GeV, as shown in column (b) of Fig. 3. With the charged Higgs boson mass in its prescribed range, a "light" neutral Higgs mass of 350 GeV is consistent with precision electroweak data!

One can increase the value for m_1 arbitrarily high and still find values of $m_{H^\pm}$ that are consistent with S and T in the allowed range. However, one eventually violates the unitarity of $Z_3 + Z_4$ (if m_1 is too high) or Z_3 alone
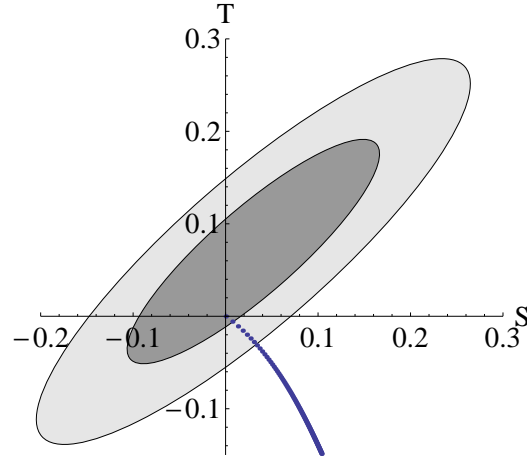
FIG. 2: The effect on S and T when m_1 is increased from 117 GeV to 500 GeV. Both S and T are zero at $m_1 = m_\phi = 117$ GeV. When m_1 reaches 175 GeV, S and T exceed the boundary of the 2 σ contour ellipse.
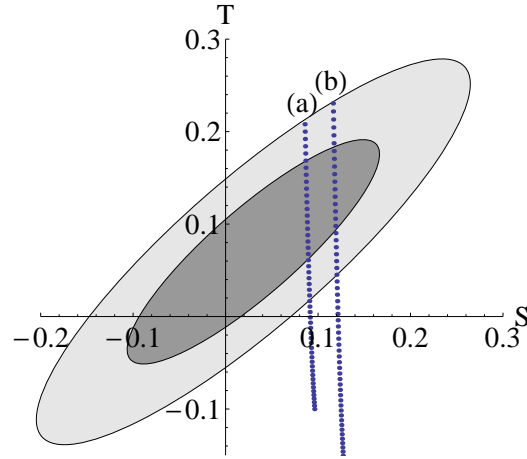
FIG. 3: The effect on S and T when $m_{H^\pm}$ is varied by increasing Z_3, for $m_1 = 350$ GeV and $m_\phi = 117$ GeV. In column (a), $Z_1 = 4$; in column (b), $Z_1 = 4\pi$. When $m_{H^\pm}$ is in the range 443–489 GeV [470–505 GeV], the points in column (a) [column (b)] fall within the 2 σ contour ellipse.

(if $m_{H^\pm}$ is too high.) As an example, by choosing $Y_2 = (50 \text{ GeV})^2$, $Z_1 = 4\pi$, $\text{Re}(Z_5\,e^{-2i\theta_{23}}) = \text{Im}(Z_5\,e^{-2i\theta_{23}})v^2 = \text{Re}(Z_6 e^{-i\theta_{23}}) = \text{Im}(Z_6 e^{-i\theta_{23}}) = 0.01$, one can adjust $Z_3 + Z_4$ to get m_1 as high as 873 GeV before violating unitarity, which gives a mass spectrum of

$$m_1 = 873 \text{ GeV}, \quad m_2 = 874 \text{ GeV}, \quad m_3 = 875 \text{ GeV}. \tag{6.4}$$

With this value of m_1, choosing Z_3 so that 716 GeV $< m_{H^\pm} <$ 750 GeV will put S and T in the upper right hand corner of the allowed 2 σ contour ellipse.[30]

We conclude that the regions of S and T allowed by precision electroweak data place significant constraints on the possible regions of the 2HDM parameter space. In the decoupling limit of the 2HDM, the only surviving constraint is on the mass of the lightest Higgs boson, which coincides with the corresponding Standard Model Higgs mass upper bound deduced from precision electroweak data. In regions of the 2HDM parameter space far from the decoupling

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[30] Note that for this choice of parameters, $m_{H^\pm} < m_1$. In fact, there are higher values of $m_{H^\pm}$ which are within the allowed ellipse, but they correspond to values of Z_3 that exceed its unitarity bound.

regime, a large chunk of the 2HDM parameter space is ruled out on the basis of the T parameter. Nevertheless, there are regions of parameter space in the non-decoupling regime, consistent with precision electroweak data, in which the lightest Higgs mass is significantly larger than the Standard Model Higgs mass upper bound.[31] This possibility is realized when large negative corrections to T from h_1 are compensated by large positive corrections to T from the other Higgs bosons of the 2HDM.

7. CONCLUSIONS

In this paper, we have employed basis-independent methods in examining the properties of the most general (CP-violating) 2HDM. Our primary aim to provide a basis-invariant characterization of a custodial-symmetric 2HDM scalar potential. Since custodial symmetry in the scalar sector of the 2HDM implies CP-conservation, we first examined in detail the basis-independent description of the most general CP-conserving 2HDM. All possible generic and special cases were examined, which depend on the values of the potentially complex quartic Higgs self-couplings in the Higgs basis. One special case where $Z_6 = Z_7 = 0$ is noteworthy, due to the fact that the CP quantum numbers of two of the three neutral Higgs states cannot be determined by the bosonic couplings of the model. This behavior can be traced to the existence of two inequivalent definitions of CP which give opposite signs for the CP-quantum numbers of each of the two neutral states. However, the ambiguity is resolved by the Higgs-fermion Yukawa interactions that uniquely selects one of the two definitions for CP and thus determines the CP quantum numbers of the two neutral states (assuming that the Yukawa interactions are CP-conserving). In fact, the Yukawa interactions could be CP-violating, even if the scalar potential *and* the Yukawa interactions respect the custodial symmetry, in which case it does not make sense to assign definite CP quantum numbers to the neutral Higgs states.

After providing a catalog of possible cases that define the CP-conserving 2HDM, we imposed custodial symmetry and determined the basis-independent condition that guarantees the presence of this symmetry. We have clarified the results of a previous analysis given in ref. [7], where it was asserted that there were two distinct cases for the custodial-symmetric scalar potential. We have demonstrated in this paper that the two cases of ref. [7] are in fact equivalent and simply correspond to two different basis choices for the scalar potential. We also showed that generically the charged Higgs boson and the CP-odd Higgs boson are mass-degenerate in the limit of a custodial symmetric scalar potential. However, in the special case of $Z_6 = Z_7 = 0$, it is possible that the charged Higgs boson and one of the CP-even Higgs bosons are mass-degenerate in the limit of a custodial symmetric scalar potential, depending on the structure of the Higgs-fermion interactions.

We have also provided a basis-independent computation of the 2HDM contributions to the oblique parameters S, T, and U. Since $T = U = 0$ in the custodial-symmetry limit, our computation provides an important check on the implications of the various mass-degeneracies noted above. The oblique parameters of the CP-violating 2HDM were analyzed numerically and found to be inconsistent with the experimental electroweak constraints over a nontrivial region of the 2HDM parameter space. Of course, there is still a significant region of the parameter space in which the oblique parameters lie within the allowed 2σ error ellipse in the S–T plane. (U is quite small over nearly the entire 2HDM parameter space, and one can set it to zero to good approximation.) In the decoupling limit, the only constraints on the 2HDM parameters are associated with the requirement that the lightest neutral Higgs boson, which is Standard Model-like in its properties, must have a mass below about 150 GeV (equivalent to the constraints of the Standard Model global fits). In the region of the 2HDM parameter space far from the decoupling regime, it is possible that the lightest neutral Higgs boson mass is significantly heavier than 150 GeV. In this case, the large negative value of T generated by the lightest neutral Higgs boson is compensated by positive corrections to T from the other physical Higgs bosons of the 2HDM.

Note Added

After this work was completed, a paper by B. Grzadkowski, M. Maniatis and J. Wudka [33] appeared that employs the formalism of gauge-invariant scalar field bilinears (cf. footnote 1) in the analysis of custodial symmetry in the 2HDM. They obtain conditions for a custodial symmetric 2HDM scalar potential that are consistent with the results obtained in this paper.

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[31] This possibility has been considered previously in ref. [32].

Appendix A: Cubic and quartic bosonic couplings in the 2HDM

The Higgs boson interactions of the 2HDM can be expressed in terms of the basis-independent $q_{k\ell}$ defined in Table I. The cubic and quartic vector-scalar couplings were obtained in ref. [2] and are reproduced below:

$$\mathscr{L}_{VVH} = \left(g m_W W_\mu^+ W^{\mu-} + \frac{g}{2c_W} m_Z Z_\mu Z^\mu \right) q_{k1} h_k$$

$$+ e m_W A^\mu (W_\mu^+ G^- + W_\mu^- G^+) - g m_Z s_W^2 Z^\mu (W_\mu^+ G^- + W_\mu^- G^+) \,, \tag{A.1}$$

$$\mathscr{L}_{VVHH} = \left[\tfrac{1}{4} g^2 W_\mu^+ W^{\mu-} + \frac{g^2}{8c_W^2} Z_\mu Z^\mu \right] h_k h_k$$

$$+ \left[\tfrac{1}{2} g^2 W_\mu^+ W^{\mu-} + e^2 A_\mu A^\mu + \frac{g^2}{c_W^2} \left(\tfrac{1}{2} - s_W^2 \right)^2 Z_\mu Z^\mu + \frac{2ge}{c_W} \left(\tfrac{1}{2} - s_W^2 \right) A_\mu Z^\mu \right] (G^+ G^- + H^+ H^-)$$

$$+ \left\{ \left(\tfrac{1}{2} eg A^\mu W_\mu^+ - \frac{g^2 s_W^2}{2c_W} Z^\mu W_\mu^+ \right) (q_{k1} G^- + q_{k2}\, e^{-i\theta_{23}} H^-) h_k + \text{h.c.} \right\} \,, \tag{A.2}$$

$$\mathscr{L}_{VHH} = \frac{g}{4c_W} \epsilon_{jk\ell} q_{\ell 1} Z^\mu h_j \overset{\leftrightarrow}{\partial}_\mu h_k - \tfrac{1}{2} g \left\{ i W_\mu^+ \left[q_{k1} G^- \overset{\leftrightarrow}{\partial}{}^\mu h_k + q_{k2} e^{-i\theta_{23}} H^- \overset{\leftrightarrow}{\partial}{}^\mu h_k \right] + \text{h.c.} \right\}$$

$$+ \left[ieA^\mu + \frac{ig}{c_W} \left(\tfrac{1}{2} - s_W^2 \right) Z^\mu \right] (G^+ \overset{\leftrightarrow}{\partial}_\mu G^- + H^+ \overset{\leftrightarrow}{\partial}_\mu H^-) \,, \tag{A.3}$$

$$\mathscr{L}_{VG} = \left[\frac{g^2}{4} W_\mu^+ W^{\mu-} + \frac{g^2}{8c_W^2} Z_\mu Z^\mu \right] G^0 G^0 + \tfrac{1}{2} g \left(W_\mu^+ G^- \overset{\leftrightarrow}{\partial}{}^\mu G^0 + W_\mu^- G^+ \overset{\leftrightarrow}{\partial}{}^\mu G^0 \right)$$

$$+ \left\{ \frac{ieg}{2} A^\mu W_\mu^+ G^- G^0 - \frac{ig^2 s_W^2}{2c_W} Z^\mu W_\mu^+ G^- G^0 + \text{h.c.} \right\} + \frac{g}{2c_W} q_{k1} Z^\mu G^0 \overset{\leftrightarrow}{\partial}_\mu h_k \,, \tag{A.4}$$

where repeated indices $j, k = 1, 2, 3$ are summed over. In obtaining the above interactions from ref. [2], we have made two simplifications. In the $W^+ W^- h_j h_k$ and $ZZ h_j h_k$ interactions, we have employed

$$q_{j1} q_{k1} + \text{Re}(q_{j2}^* q_{k2}) = \delta_{jk} \,, \qquad \text{for} \ \ j, k = 1, 2, 3. \tag{A.5}$$

In the $Z h_j h_k$ interactions $(j, k = 1, 2, 3)$, we have made use of the identity

$$\text{Im}(q_{j2}^* q_{k2}) = \sum_{\ell=1}^{3} \epsilon_{jk\ell} q_{\ell 1} \,. \tag{A.6}$$

Likewise, a basis-independent form for the cubic and quartic scalar self-interactions has been obtained in ref. [2] and are reproduced below. In listing the scalar self-interactions, it is convenient to include terms involving the Goldstone

field by denoting $h_4 \equiv G^0$.

$$\mathcal{V}_3 = \tfrac{1}{2}v\, h_j h_k h_\ell \Big[q_{j1}q_{k1}^* \mathrm{Re}(q_{\ell 1})Z_1 + q_{j2}q_{k2}^* \mathrm{Re}(q_{\ell 1})(Z_3 + Z_4) + \mathrm{Re}(q_{j1}^* q_{k2} q_{\ell 2} Z_5\, e^{-2i\theta_{23}})$$

$$+ \mathrm{Re}\left([2q_{j1} + q_{j1}^*]q_{k1}^* q_{\ell 2} Z_6\, e^{-i\theta_{23}}\right) + \mathrm{Re}(q_{j2}^* q_{k2} q_{\ell 2} Z_7\, e^{-i\theta_{23}}) \Big]$$

$$+ v\, h_k G^+ G^- \Big[\mathrm{Re}(q_{k1})Z_1 + \mathrm{Re}(q_{k2}\, e^{-i\theta_{23}} Z_6) \Big] + v\, h_k H^+ H^- \Big[\mathrm{Re}(q_{k1})Z_3 + \mathrm{Re}(q_{k2}\, e^{-i\theta_{23}} Z_7) \Big]$$

$$+ \tfrac{1}{2}v\, h_k \Big\{ G^- H^+ e^{i\theta_{23}} \left[q_{k2}^* Z_4 + q_{k2}\, e^{-2i\theta_{23}} Z_5 + 2\mathrm{Re}(q_{k1})Z_6\, e^{-i\theta_{23}} \right] + \text{h.c.} \Big\} \,, \tag{A.7}$$

$$\mathcal{V}_4 = \tfrac{1}{8} h_j h_k h_l h_m \Big[q_{j1}q_{k1}q_{\ell 1}^* q_{m1}^* Z_1 + q_{j2}q_{k2}q_{\ell 2}^* q_{m2}^* Z_2 + 2q_{j1}q_{k1}^* q_{\ell 2}q_{m2}^*(Z_3 + Z_4)$$

$$+ 2\mathrm{Re}(q_{j1}^* q_{k1}^* q_{\ell 2}q_{m2} Z_5\, e^{-2i\theta_{23}}) + 4\mathrm{Re}(q_{j1}q_{k1}^* q_{\ell 1}^* q_{m2} Z_6\, e^{-i\theta_{23}}) + 4\mathrm{Re}(q_{j1}^* q_{k2}q_{\ell 2}q_{m2}^* Z_7\, e^{-i\theta_{23}}) \Big]$$

$$+ \tfrac{1}{2} h_j h_k G^+ G^- \Big[q_{j1}q_{k1}^* Z_1 + q_{j2}q_{k2}^* Z_3 + 2\mathrm{Re}(q_{j1}q_{k2} Z_6\, e^{-i\theta_{23}}) \Big]$$

$$+ \tfrac{1}{2} h_j h_k H^+ H^- \Big[q_{j2}q_{k2}^* Z_2 + q_{j1}q_{k1}^* Z_3 + 2\mathrm{Re}(q_{j1}q_{k2} Z_7\, e^{-i\theta_{23}}) \Big]$$

$$+ \tfrac{1}{2} h_j h_k \Big\{ G^- H^+ e^{i\theta_{23}} \left[q_{j1}q_{k2}^* Z_4 + q_{j1}^* q_{k2} Z_5\, e^{-2i\theta_{23}} + q_{j1}q_{k1}^* Z_6\, e^{-i\theta_{23}} + q_{j2}q_{k2}^* Z_7\, e^{-i\theta_{23}} \right] + \text{h.c.} \Big\}$$

$$+ \tfrac{1}{2} Z_1 G^+ G^- G^+ G^- + \tfrac{1}{2} Z_2 H^+ H^- H^+ H^- + (Z_3 + Z_4) G^+ G^- H^+ H^- + \tfrac{1}{2} Z_5 H^+ H^+ G^- G^-$$

$$+ \tfrac{1}{2} Z_5^* H^- H^- G^+ G^+ + G^+ G^- (Z_6 H^+ G^- + Z_6^* H^- G^+) + H^+ H^- (Z_7 H^+ G^- + Z_7^* H^- G^+) \,, \tag{A.8}$$

summing over j, k, ℓ, $m = 1, 2, 3, 4$. Note that $\mathrm{Re}(q_{k1}) = q_{k1}$ for $k = 1, 2, 3$, whereas $\mathrm{Re}(q_{41}) = 0$.

One can easily verify that if $q_{k1} = \pm 1$ and $q_{k2} = 0$ for a fixed value of $k = 1, 2$ or 3. then it follows that the couplings of the neutral Higgs field, $\pm h_k$, are precisely those of the Standard Model Higgs boson.

Appendix B: Neutral Higgs masses and invariant mixing angles

The neutral Higgs mass eigenstates are denoted by h_k ($k = 1, 2, 3$). The corresponding squared-masses are obtained by solving the characteristic equation of the neutral Higgs squared-mass matrix, $\mathcal{M}^2$ [see eq. (2.17)],

$$\det(\mathcal{M} - x\, \mathbb{1}_{3\times 3}) = -x^3 + \mathrm{Tr}(\mathcal{M})\, x^2 - \tfrac{1}{2}\left[(\mathrm{Tr}\mathcal{M})^2 - \mathrm{Tr}(\mathcal{M}^2)\right] x + \det(\mathcal{M}) = 0 \,, \tag{B.1}$$

where $\mathbb{1}_{3\times 3}$ is the 3×3 identity matrix and

$$\mathrm{Tr}(\mathcal{M}) = 2Y_2 + (Z_1 + Z_3 + Z_4)v^2 \,,$$
$$\mathrm{Tr}(\mathcal{M}^2) = Z_1^2 v^4 + \tfrac{1}{2}v^4 \left[(Z_3 + Z_4)^2 + |Z_5|^2 + 4|Z_6|^2\right] + 2Y_2[Y_2 + (Z_3 + Z_4)v^2] \,,$$
$$\det(\mathcal{M}) = \tfrac{1}{4}\Big\{ Z_1 v^6[(Z_3 + Z_4)^2 - |Z_5|^2] - 2v^4[2Y_2 + (Z_3 + Z_4)v^2]|Z_6|^2$$
$$+ 4Y_2 Z_1 v^2[Y_2 + (Z_3 + Z_4)v^2] + 2v^6 \mathrm{Re}(Z_5^* Z_6^2) \Big\} \,. \tag{B.2}$$

In the general (CP-violating) case, the analytic expressions for the squared-masses are quite cumbersome, when expressed solely in terms of the scalar potential parameters. In ref. [2], a more convenient expression for the neutral Higgs squared-masses was derived in terms of the Z_i and invariant mixing angles,

$$m_k^2 = |q_{k2}|^2 A^2 + v^2 \left[q_{k1}^2 Z_1 + \mathrm{Re}(q_{k2})\, \mathrm{Re}(q_{k2} Z_5\, e^{-2i\theta_{23}}) + 2q_{k1} \mathrm{Re}(q_{k2} Z_6\, e^{-i\theta_{23}}) \right] \,, \tag{B.3}$$

where $m_k^2 \equiv m_{h_k}^2$ (for $k = 1, 2, 3$) and the basis-invariant q_{ki} are given in Table I.

In ref. [2], we also obtained a set of equations that determine the neutral Higgs mixing angles:[32]

$$s_{13}\text{Re}(Z_6\,e^{-i\theta_{23}}) = \tfrac{1}{2}c_{13}\text{Im}(Z_5\,e^{-2i\theta_{23}})\,, \tag{B.4}$$

$$(Z_1 - A^2/v^2)s_{13}c_{13} = (c_{13}^2 - s_{13}^2)\text{Im}(Z_6\,e^{-i\theta_{23}})\,, \tag{B.5}$$

$$(c_{12}^2 - s_{12}^2)\big[c_{13}\text{Re}(Z_6\,e^{-i\theta_{23}}) + \tfrac{1}{2}s_{13}\text{Im}(Z_5\,e^{-2i\theta_{23}})\big] = s_{12}c_{12}\big[\text{Re}(Z_5\,e^{-2i\theta_{23}}) - (Z_1 - A^2/v^2)c_{13}^2$$
$$-2s_{13}c_{13}\text{Im}(Z_6\,e^{-i\theta_{23}})\big]\,, \tag{B.6}$$

where

$$A^2 \equiv Y_2 + \tfrac{1}{2}\big[Z_3 + Z_4 - \text{Re}(Z_5\,e^{-2i\theta_{23}})\big]v^2\,. \tag{B.7}$$

Eqs. (B.3)–(B.6) can be used to derive the following results:

$$\text{Re}(Z_6\,e^{-i\theta_{23}})\,v^2 = c_{13}s_{12}c_{12}(m_2^2 - m_1^2)\,, \tag{B.8}$$

$$\text{Im}(Z_6\,e^{-i\theta_{23}})\,v^2 = s_{13}c_{13}(c_{12}^2 m_1^2 + s_{12}^2 m_2^2 - m_3^2)\,, \tag{B.9}$$

$$\text{Re}(Z_5\,e^{-2i\theta_{23}})\,v^2 = (s_{12}^2 - s_{13}^2 c_{12}^2)m_1^2 + (c_{12}^2 - s_{12}^2 s_{13}^2)m_2^2 - c_{13}^2 m_3^2\,, \tag{B.10}$$

$$\text{Im}(Z_5\,e^{-2i\theta_{23}})\,v^2 = 2s_{13}s_{12}c_{12}(m_2^2 - m_1^2)\,. \tag{B.11}$$

The following identity will also prove useful,

$$\text{Im}(Z_5^* Z_6^2) = 2\,\text{Re}(Z_5 e^{-2i\theta_{23}})\,\text{Re}(Z_6\,e^{-i\theta_{23}})\,\text{Im}(Z_6\,e^{-i\theta_{23}})$$
$$-\text{Im}(Z_5 e^{-2i\theta_{23}})\big\{[\text{Re}(Z_6\,e^{-i\theta_{23}})]^2 - [\text{Im}(Z_6\,e^{-i\theta_{23}})]^2\big\}\,. \tag{B.12}$$

Using the results of eqs. (B.8)–(B.12) it then follows that:

$$v^6\text{Im}(Z_5^* Z_6^2) = s_{13}c_{13}^2\sin 2\theta_{12}\,(m_2^2 - m_1^2)(m_3^2 - m_1^2)(m_3^2 - m_2^2)\,. \tag{B.13}$$

Appendix C: Basis-Independent treatment of the CP-conserving 2HDM

In the CP-conserving Higgs sector, two of the neutral Higgs bosons, h^0 and H^0 (with $m_{h^0} < m_{H^0}$) are CP-even and one neutral Higgs boson, A^0, is CP-odd. Basis-independent conditions for a CP-conserving bosonic sector have been given in refs. [1, 10, 11, 34]. In ref. [1], these conditions were recast into the form given by eq. (3.1). Since the Higgs masses and mixing angles do not depend on Z_7, we focus on the implications of the condition $\text{Im}[Z_5^* Z_6^2] = 0$ for the structure of the neutral Higgs squared-mass matrix and the invariant mixing angles.

1. The CP-conserving limit: $Z_6 \neq 0$

If $Z_6 \neq 0$, then eqs. (B.8) and (B.9) imply that $c_{13} \neq 0$. Suppose that the three neutral Higgs masses are non-degenerate. Under the latter assumption, if the CP-conserving condition $\text{Im}(Z_5^* Z_6^2) = 0$ holds, then eq. (B.13) implies that $s_{13}s_{12}c_{12} = 0$. We examine the two resulting cases in turn.[33]

Case I: $s_{13} = 0$. Then, eqs. (B.4)–(B.9) imply that:

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

---

[32] Denoting the quadratic terms in the scalar potential by $m_{H^\pm}^2 H^+ H^- + \tfrac{1}{2}v^2 \sum_{j,k} C_{jk} h_j h_k$, it follows that $C_{jk} = 0$ for $j \neq k$. This provides three conditions, which yield eqs. (B.4)–(B.6).

[33] Note that setting eq. (B.12) to zero determines $\text{Re}(Z_5\,e^{-2i\theta_{23}})$ in terms of $\text{Im}(Z_5\,e^{-2i\theta_{23}})$, $\text{Re}(Z_6\,e^{-i\theta_{23}})$ and $\text{Im}(Z_6\,e^{-i\theta_{23}})$. However, this is not sufficient to impose the conditions given in Cases I and II. This is because the diagonalization of the neutral Higgs squared-mass matrix yields an extra (basis-dependent) condition that fixes the value of θ_{23}.

Case II: $s_{12}c_{12} = 0$. Then, eqs. (B.8) and (B.13) imply that:

$$\text{Im}(Z_5\, e^{-2i\theta_{23}}) = \text{Re}(Z_6\, e^{-i\theta_{23}}) = 0\,. \tag{C.2}$$

In Section 3.1, Case II is further broken down into two subcases (a) and (b) corresponding to $s_{12} = 0$ and $c_{12} = 0$, respectively. The three cases I, IIa and IIb simply correspond to three possible mass orderings of the neutral Higgs bosons—the CP-even h^0 and H^0 (where $m_{h^0} < m_{H^0}$ by definition) and the CP-odd A^0.

It is convenient to define the invariant angle $\phi \equiv \theta_6 - \theta_{23}$, where $\theta_6 \equiv \arg Z_6$. That is,

$$\text{Re}(Z_6\, e^{-i\theta_{23}}) \equiv |Z_6|\cos\phi\,, \qquad \text{Im}(Z_6\, e^{-i\theta_{23}}) \equiv |Z_6|\sin\phi\,. \tag{C.3}$$

Then, Cases I and II correspond to $\sin\phi = 0$ and $\cos\phi = 0$, respectively. That is, if CP is conserved then $\sin 2\phi = 0$. Note that the converse is not necessarily valid. In particular,

$$\text{Im}(Z_5\, e^{-2i\theta_{23}}) = \frac{1}{|Z_6|^2}\left[\text{Re}(Z_5^* Z_6^2)\sin 2\phi - \text{Im}(Z_5^* Z_6^2)\cos 2\phi\right]\,. \tag{C.4}$$

Thus, if $\sin 2\phi = 0$ and $\text{Im}(Z_5\, e^{-2i\theta_{23}}) \neq 0$, then the Higgs sector violates CP.

The quantum numbers of the neutral Higgs bosons can be determined from the form of the Higgs self-couplings. For example, noting that a charged Goldstone boson pair is necessarily CP-even, the couplings of $G^+ G^-$ to the neutral Higgs bosons can be used to identify the CP-even scalars. In Appendix A, the following couplings are given:

$$G^+ G^- h_1: \qquad c_{12}c_{13}Z_1 - s_{12}\text{Re}(Z_6\, e^{-i\theta_{23}}) + c_{12}s_{13}\text{Im}(Z_6\, e^{-i\theta_{23}})\,, \tag{C.5}$$

$$G^+ G^- h_2: \qquad s_{12}c_{13}Z_1 + c_{12}\text{Re}(Z_6\, e^{-i\theta_{23}}) + s_{12}s_{13}\text{Im}(Z_6\, e^{-i\theta_{23}})\,, \tag{C.6}$$

$$G^+ G^- h_3: \qquad s_{13}Z_1 - c_{13}\text{Im}(Z_6\, e^{-i\theta_{23}})\,, \tag{C.7}$$

where the mixing angles are defined such that $m_{h_1} \leq m_{h_2} \leq m_{h_3}$. Since one of the three neutral states is CP-odd, its coupling to $G^+ G^-$ must vanish. Taking Z_1 and Z_6 as independent and non-vanishing,[34]

$$\text{if } h_1 \text{ is CP odd}, \qquad c_{12} = \text{Re}(Z_6\, e^{-i\theta_{23}}) = \cos\phi = 0\,, \tag{C.8}$$

$$\text{if } h_2 \text{ is CP odd}, \qquad s_{12} = \text{Re}(Z_6\, e^{-i\theta_{23}}) = \cos\phi = 0\,, \tag{C.9}$$

$$\text{if } h_3 \text{ is CP odd}, \qquad s_{13} = \text{Im}(Z_6\, e^{-i\theta_{23}}) = \sin\phi = 0\,, \tag{C.10}$$

which reproduces Cases I and II [eqs. (C.1) and (C.2)] for non-degenerate neutral Higgs masses.

The masses of the three neutral Higgs bosons can be evaluated explicitly using eqs. (B.1) and (B.2). In evaluating $\det(\mathcal{M})$, we employ the condition $\text{Im}(Z_5^* Z_6^2) = 0$, which implies that $[\text{Re}(Z_5^* Z_6^2)]^2 = |Z_5|^2\,|Z_6|^4$, and leads to two possible cases:

$$\text{Re}(Z_5^* Z_6^2) = \varepsilon_{56}|Z_5|\,|Z_6|^2\,, \qquad \varepsilon_{56} \equiv \pm 1\,. \tag{C.11}$$

In both cases, eq. (B.1) factors into a product of a linear and a quadratic polynomial. Solving for the roots, the resulting neutral Higgs squared-masses are given by eqs. (3.16) and (3.17), where the CP-odd state is identified according to the results of eq. (B.3) and eqs. (C.8)–(C.10).

2. Degenerate masses in the CP-conserving limit with $Z_6 \neq 0$

So far, we have working under the assumption that the three Higgs masses are unequal. However, it is also possible that two of the Higgs bosons are mass-degenerate.[35] In this case, it follows from eq. (B.13) that $\text{Im}(Z_5^* Z_6^2) = 0$, independently of the mixing angles (some of which may not be well-defined in the mass-degenerate limit). If $Z_5 = 0$ and $Z_6 \neq 0$, then eqs. (3.16) and (3.17) imply that the three three neutral Higgs masses are distinct. Hence, in what follows we assume that $Z_5 \neq 0$, in which case A^0 and one of the CP-even scalars are degenerate in mass if:[36]

$$Z_1 = Y_2/v^2 + \tfrac{1}{2}(Z_3 + Z_4 - \varepsilon_{56}|Z_5|) + \frac{|Z_6|^2}{\varepsilon_{56}|Z_5|} \qquad \text{and} \qquad \text{Im}(Z_5^* Z_6^2) = 0\,. \tag{C.12}$$

---

[34] Similar conclusions can be obtained by considering the ZZh_i, the Zh_ih_j, and the $ZG^0 h_i$ couplings.

[35] Under the assumption $Z_6 \neq 0$, it is not possible to have three mass-degenerate neutral Higgs bosons.

[36] One can also verify the condition for degenerate roots directly from eq. (B.1). The cubic equation $z^3 + a_2 z^2 + a_1 z + a_0$ has (at least) two degenerate roots if and only if [35]

$$\left[\tfrac{1}{3}a_1 - \tfrac{1}{9}a_2^2\right]^3 + \left[\tfrac{1}{6}(a_1 a_2 - 3a_0) - \tfrac{1}{27}a_2^3\right]^2 = 0\,.$$

With a little help from Mathematica, one can show that by imposing the above equation, eq. (C.12) is satisfied.

Inserting this result for Z_1 back into eqs. (3.16) and (3.17) then yields:

$$m_{h^0}^2 = m_{A^0}^2 = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 - |Z_5|)v^2 \,, \tag{C.13}$$

$$m_{H^0}^2 = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 + |Z_5|)v^2 + \frac{|Z_6|^2 v^2}{|Z_5|} \,, \qquad \text{for} \quad \varepsilon_{56} = +1 \,, \tag{C.14}$$

and

$$m_{h^0}^2 = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 - |Z_5|)v^2 - \frac{|Z_6|^2 v^2}{|Z_5|} \,, \tag{C.15}$$

$$m_{H^0}^2 = m_{A^0}^2 = Y_2 + \tfrac{1}{2}(Z_3 + Z_4 + |Z_5|)v^2 \,, \qquad \text{for} \quad \varepsilon_{56} = -1 \,. \tag{C.16}$$

In the mass-degenerate case, the mixing angle θ_{23} and the corresponding invariant angle ϕ are no longer well-defined, as one can redefine the mixing angles by rotating within the degenerate subspace. Hence, the choice of $\sin 2\phi$ is arbitrary. However, because CP is conserved in the neutral Higgs sector, the structure of the Higgs interactions guarantees that there exists one linear combination of the mass-degenerate neutral Higgs states that is CP-even and an orthogonal linear combination that is CP-odd. The latter defines the relevant mixing angle, θ_{12} in Case I and θ_{13} in Case II, respectively. In particular, the identification of eigenstates of definite CP quantum numbers imposes the constraint $s_{13} = s_{12}c_{12} = \sin 2\phi = 0$, and the conditions of Cases I and II continue to hold. A summary of the basis-independent conditions for CP-invariance, under the assumption that $Z_6 \neq 0$, along with the identification of the CP quantum numbers of the three neutral Higgs states can be found in Table II.

In Section 4.1.2, we determined the basis-independent conditions for a custodial symmetric scalar potential. In the case of $Z_6 \neq 0$, the relevant condition is $Z_4 = \epsilon_{56}|Z_5|$ [cf. eq. (4.46)]. Using eqs. (4.49), (C.13) and (C.16), we conclude that when eq. (C.12) holds, the custodial symmetric scalar potential yields two neutral Higgs bosons, one CP-even and one CP-odd, that are both degenerate in mass with the charged Higgs boson.

3. The CP-conserving Limit: $Z_6 = 0$

The case where $Z_6 = 0$ (with $Z_5 \neq 0$) merits special attention. In this case, eqs. (B.4)–(B.6) simplify to:

$$c_{13}\mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = 0 \,, \tag{C.17}$$

$$(Z_1 v^2 - A^2)s_{13}c_{13} = 0 \,, \tag{C.18}$$

$$\tfrac{1}{2}s_{13}(c_{12}^2 - s_{12}^2)\mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = s_{12}c_{12}\left[\mathrm{Re}(Z_5\, e^{-2i\theta_{23}}) - (Z_1 - A^2/v^2)c_{13}^2\right] \,. \tag{C.19}$$

First we consider cases in which the three neutral Higgs masses are non-degenerate. Then in the CP-conserving limit, eq. (B.13) implies that $s_{13}s_{12}c_{12} = 0$. If $c_{13}s_{13} \neq 0$, then eqs. (C.17) and (C.18) yield $\mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = 0$ and $Z_1 v^2 = A^2$. In this case $\mathrm{Re}(Z_5\, e^{-2i\theta_{23}}) = \pm|Z_5|$ and $A^2 = Y_2 + \tfrac{1}{2}v^2(Z_3 + Z_4 \mp |Z_5|)$, where both sign choices are possible. For either sign choice, eqs. (3.24)–(3.26) imply that two of the neutral Higgs bosons are degenerate in mass, which contradicts our initial assumption. Thus, if the Higgs bosons are non-degenerate, then eq. (C.18) implies that either $s_{13} = 0$ or $c_{13} = 0$. If $s_{13} = 0$ then eqs. (C.17) and (C.18) yield either $s_{12}c_{12} = 0$ or $\mathrm{Re}(Z_5\, e^{-2i\theta_{23}}) = Z_1 - A^2/v^2$. However, in the latter case one again finds that two of the neutral Higgs bosons are degenerate in mass, which again contradicts our initial assumption. Thus, in the case of non-degenerate neutral Higgs masses, there are three cases to consider:

Case I′: $s_{13} = s_{12} = \mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = 0$. This is a combination of the previous Cases I and IIa.

Case II′: $s_{13} = c_{12} = \mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = 0$. This is a combination of the previous Cases I and IIb.

When $Z_6 = 0$ and CP is conserved, a new third possibility arises in which $c_{13} = 0$. In this case, eq. (C.19) yields $\tfrac{1}{2}s_{13}(c_{12}^2 - s_{12}^2)\mathrm{Im}(Z_5\, e^{-2i\theta_{23}}) = s_{12}c_{12}\mathrm{Re}(Z_5\, e^{-2i\theta_{23}})$, where $s_{13} = \pm 1$. Following the convention specified in Table I, we choose $s_{13} = -1$. In this convention, $\theta_{12} + \theta_{23}$ is indeterminate, and the quantity

$$\overline{\theta}_{23} \equiv \theta_{23} - \theta_{12} \,, \tag{C.20}$$

plays the role of θ_{23}. We designate this new case

Case III′: $c_{13} = \mathrm{Im}(Z_5\, e^{-2i\overline{\theta}_{23}}) = 0$.

To determine the CP-quantum numbers of the h_k, we first examine the $G^+G^-h_k$ couplings when $Z_6 = 0$ [cf. eqs. (C.5)–(C.7)]:

$$G^+G^-h_1: \qquad c_{12}c_{13}Z_1\,, \tag{C.21}$$

$$G^+G^-h_2: \qquad s_{12}c_{13}Z_1\,, \tag{C.22}$$

$$G^+G^-h_3: \qquad s_{13}Z_1\,, \tag{C.23}$$

One of these three couplings is non-vanishing in Cases I$'$, II$'$ and III$'$, which implies that the corresponding neutral Higgs state (h_k for $k = 1, 2$ or 3) is CP-even. Moreover, in this case, $q_{k1} = \pm 1$ and $q_{k2} = 0$, which implies that the couplings of the neutral Higgs field $\pm h_k$ are precisely those of the Standard Model Higgs boson. Henceforth, we identify the Standard Model–like CP-even neutral Higgs field by h_1^0. We then use eq. (B.3) to obtain $m_{h_1^0}^2 = Z_1 v^2$ [cf. eq. (3.24)]. If we order the states h_i such that $m_{h_1} < m_{h_2} < m_{h_3}$, then the three cases I$'$, II$'$ and III$'$ above correspond to the three possible mass orderings of h_1^0.

By examining the non-vanishing Zh_ih_j couplings, one immediately concludes that the relative CP quantum number of the other two neutral Higgs bosons is negative. However, there is no unique assignment for the individual CP quantum numbers if $Z_7 = \rho^Q = 0$. For simplicity, we assume that $Z_7 \neq 0$.[37] The following identity, analogous to eq. (B.13), will also prove useful:

$$\mathrm{Im}(Z_5^* Z_7^2) = 2\,\mathrm{Re}(Z_5 e^{-2i\theta_{23}})\,\mathrm{Re}(Z_7\,e^{-i\theta_{23}})\,\mathrm{Im}(Z_7\,e^{-i\theta_{23}})$$
$$- \mathrm{Im}(Z_5 e^{-2i\theta_{23}})\left\{[\mathrm{Re}(Z_7\,e^{-i\theta_{23}})]^2 - [\mathrm{Im}(Z_7\,e^{-i\theta_{23}})]^2\right\}\,. \tag{C.24}$$

Under the assumption of a CP-conserving Higgs sector, we impose the condition $\mathrm{Im}(Z_5^* Z_7^2) = 0$, which implies that $[\mathrm{Re}(Z_5^* Z_7^2)]^2 = |Z_5|^2\,|Z_7|^4$, and leads to two possible cases:

$$\mathrm{Re}(Z_5^* Z_7^2) = \varepsilon_{57}|Z_5||Z_7|^2\,, \qquad \varepsilon_{57} = \pm 1\,. \tag{C.25}$$

In Cases I$'$ and II$'$, $\mathrm{Im}(Z_5\,e^{-2i\theta_{23}}) = 0$, whereas $\mathrm{Im}(Z_5\,e^{-2i\overline{\theta}_{23}}) = 0$ in Case III$'$. Then, eq. (C.24) yields:

$$\text{Case I}', \text{II}': \qquad \mathrm{Re}(Z_7\,e^{-i\theta_{23}})\,\mathrm{Im}(Z_7\,e^{-i\theta_{23}}) = 0\,. \tag{C.26}$$

$$\text{Case III}': \qquad \mathrm{Re}(Z_7\,e^{-i\overline{\theta}_{23}})\,\mathrm{Im}(Z_7\,e^{-i\overline{\theta}_{23}}) = 0\,. \tag{C.27}$$

We can use the $H^+H^-h_k$ couplings to determine the CP-quantum numbers of the other two neutral Higgs bosons. In cases I$'$ and II$'$,

$$H^+H^-h_1: \qquad c_{12}c_{13}Z_3 - s_{12}\mathrm{Re}(Z_7\,e^{-i\theta_{23}}) + c_{12}s_{13}\mathrm{Im}(Z_7\,e^{-i\theta_{23}})\,, \tag{C.28}$$

$$H^+H^-h_2: \qquad s_{12}c_{13}Z_3 + c_{12}\mathrm{Re}(Z_7\,e^{-i\theta_{23}}) + s_{12}s_{13}\mathrm{Im}(Z_7\,e^{-i\theta_{23}})\,, \tag{C.29}$$

$$H^+H^-h_3: \qquad s_{13}Z_3 - c_{13}\mathrm{Im}(Z_7\,e^{-i\theta_{23}})\,. \tag{C.30}$$

In Case III$'$, these couplings simplify to:

$$H^+H^-h_1: \qquad -\mathrm{Im}(Z_7\,e^{-i\overline{\theta}_{23}})\,, \tag{C.31}$$

$$H^+H^-h_2: \qquad \mathrm{Re}(Z_7\,e^{-i\overline{\theta}_{23}})\,, \tag{C.32}$$

$$H^+H^-h_3: \qquad -Z_3\,. \tag{C.33}$$

Since one of the three neutral states is CP-odd, its coupling to H^+H^- must vanish. Taking Z_3 and Z_7 as independent and non-vanishing, we can identify the CP-odd Higgs boson. Hence, using eqs. (C.28)–(C.33),

- if h_1 is CP-odd, then either

$$s_{13} = c_{12} = \mathrm{Re}(Z_7\,e^{-i\theta_{23}}) = 0 \quad \text{[Case II}'\text{b]} \quad \text{or} \quad c_{13} = \mathrm{Im}(Z_7\,e^{-i\overline{\theta}_{23}}) = 0 \quad \text{[Case III}'\text{a]}\,, \tag{C.34}$$

- if h_2 is CP-odd, then either

$$s_{13} = s_{12} = \mathrm{Re}(Z_7\,e^{-i\theta_{23}}) = 0 \quad \text{[Case I}'\text{b]} \quad \text{or} \quad c_{13} = \mathrm{Re}(Z_7\,e^{-i\overline{\theta}_{23}}) = 0 \quad \text{[Case III}'\text{b]}\,, \tag{C.35}$$

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[37] If $Z_7 = 0$ but $\rho^Q \neq 0$, then our analysis still goes through with Z_7 replaced by ρ^{Q*} ($Q = U$, D or E).

- if h_3 is CP-odd, then either

$$s_{13} = s_{12} = \mathrm{Im}(Z_7\, e^{-i\theta_{23}}) = 0 \qquad \text{[Case I$'$a]} \qquad \text{or} \qquad s_{13} = c_{12} = \mathrm{Im}(Z_7\, e^{-i\theta_{23}}) = 0 \qquad \text{[Case II$'$a]} . \qquad (C.36)$$

These correspond to six possible mass orderings of h_1, h_2 and h_3 in Cases I$'$, II$'$ and III$'$.

We previously identified the CP-even state h_1^0, whose couplings coincide with those of the Standard Model Higgs boson. Using eq. (B.3), the squared-masses of the remaining two neutral Higgs bosons (a CP-even state h_2^0 and a CP-odd state A^0) are given by eqs. (3.25) and (3.26), after making use of eq. (3.22) for Cases I$'$ and II$'$ (and replacing θ_{23} with $\overline{\theta}_{23}$ for Case III$'$). We identify the states h_1^0 and h_2^0 with h^0 and H^0 or vice versa, depending on the mass-ordering. If $Z_7 = 0$, then ε_{57} is not well-defined (since in the real basis, the sign of Z_5 can be flipped by transforming $H_2 \to iH_2$). In this case, the individual CP-quantum numbers of h_2^0 and A^0 are not fixed by the interactions of the Higgs boson/gauge boson sector. The corresponding masses are given in eq. (3.28), which can be derived by directly solving the characteristic equation of the neutral Higgs squared-mass matrix [cf. eq. (B.1)].

A summary of the basis-independent conditions for CP-invariance, under the assumption that $Z_6 = 0$ and the Higgs masses are non-degenerate, along with the identification of the CP quantum numbers of the three neutral Higgs states can be found in Table VI.

4. Degenerate masses in the CP-conserving limit with $Z_6 = 0$

It is possible to have two mass-degenerate neutral Higgs bosons in the 2HDM with $Z_6 = 0$, for special choices of Z_1. If Z_1 satisfies

$$Z_1 = Y_2/v^2 + \tfrac{1}{2}(Z_3 + Z_4 - \varepsilon_{57}|Z_5|)v^2 , \qquad (C.37)$$

then eqs. (3.24) and (3.26) yield $m_{h_1^0} = m_{A^0}$ [this is the analogue of eq. (C.12)]. Likewise, if Z_1 satisfies

$$Z_1 = Y_2/v^2 + \tfrac{1}{2}(Z_3 + Z_4 + \varepsilon_{57}|Z_5|)v^2 , \qquad (C.38)$$

then eqs. (3.24) and (3.25) yield $m_{h_1^0} = m_{h_2^0}$ (this has no analogue with any of the $Z_6 \neq 0$ cases). In the presence of mass degeneracies, one must reconsider the definition of the mixing angles θ_{12} and θ_{13}. As in the discussion below eq. (C.16), if two neutral scalar states of opposite CP quantum number are mass degenerate, then the structure of the Higgs interactions guarantees that there exists one linear combination of the mass-degenerate neutral Higgs states that is CP-even and an orthogonal linear combination that is CP-odd. If the two neutral mass-degenerate scalar states are CP-even, then there exists one linear combination whose properties coincide precisely with those of the Standard Model Higgs boson. We designate this scalar field by h_1^0 and the orthogonal linear combination by h_2^0. In light of these remarks, the results of Table VI continue to hold even in the mass-degenerate case.

However, there are three new cases that arise if two of the neutral Higgs fields are mass-degenerate, which are not accounted for by Cases I$'$, II$'$ and III$'$. These exceptional cases correspond to the omitted cases described below eq. (C.19). In particular, mass-degeneracies arise for a special choice of Z_1 in following cases:

Case IV$'$: $s_{13} = \mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$ and $s_{12}c_{12} \neq 0$. In this case, eq. (C.19) yields

$$Z_1 = A^2/v^2 + \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) = Y_2/v^2 + \tfrac{1}{2}\left[Z_3 + Z_4 + \mathrm{Re}(Z_5 e^{-2i\theta_{23}})\right] , \qquad (C.39)$$

where we have used the definition of A^2 given in eq. (B.7). The quantity $\mathrm{Re}(Z_5 e^{-2i\theta_{23}})$ is fixed by eq. (3.22).

Case V$'$: $c_{12} = \mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$ and $s_{13}c_{13} \neq 0$. In this case, eq. (C.18) yields

$$Z_1 = A^2/v^2 = Y_2/v^2 + \tfrac{1}{2}\left[Z_3 + Z_4 - \mathrm{Re}(Z_5 e^{-2i\theta_{23}})\right] . \qquad (C.40)$$

Case VI$'$: $s_{12} = \mathrm{Im}(Z_5 e^{-2i\theta_{23}}) = 0$ and $s_{13}c_{13} \neq 0$. In this case, eq. (C.18) yields

$$Z_1 = A^2/v^2 = Y_2/v^2 + \tfrac{1}{2}\left[Z_3 + Z_4 - \mathrm{Re}(Z_5 e^{-2i\theta_{23}})\right] . \qquad (C.41)$$

Once again, we find that $m_{h_1^0} = m_{A^0}$ if eq. (C.37) is satisfied and $m_{h_1^0} = m_{h_2^0}$ if eq. (C.38) is satisfied.

To identify the CP quantum numbers of the neutral Higgs mass eigenstates, we first examine the $G^+G^- h_k$ couplings given in eqs. (C.21)–(C.23) in order to identify the mass-degenerate state h_1^0, which is defined below eq. (C.38) to be the linear combination of mass-degenerate neutral Higgs fields whose interactions coincide with that of the Standard

Model Higgs boson . The CP quantum numbers of the orthogonal linear combination of mass-degenerate neutral Higgs fields and the third non-degenerate state can be obtained by examining the $H^+H^-h_k$ couplings given in eqs. (C.28)–(C.30).

For example, in Case IV$'$, $s_{13} = 0$ which yields

$$H^+H^-h_1 : \qquad c_{12}Z_3 - s_{12}\text{Re}(Z_7\,e^{-i\theta_{23}}), \qquad m_{h_1}^2 = Z_1 v^2, \tag{C.42}$$

$$H^+H^-h_2 : \qquad s_{12}Z_3 + c_{12}\text{Re}(Z_7\,e^{-i\theta_{23}}), \qquad m_{h_2}^2 = Z_1 v^2, \tag{C.43}$$

$$H^+H^-h_3 : \qquad -\text{Im}(Z_7\,e^{-i\theta_{23}}), \qquad m_{h_3}^2 = \left[Z_1 - \text{Re}(Z_5 e^{-2i\theta_{23}})\right]v^2. \tag{C.44}$$

Since h_1 and h_2 are degenerate, we can redefine new linear combinations to obtain:

$$H^+H^-(c_{12}h_1 + s_{12}h_2) : \qquad c_{12}Z_3, \tag{C.45}$$

$$H^+H^-(c_{12}h_2 - s_{12}h_1) : \qquad \text{Re}(Z_7\,e^{-i\theta_{23}}), \tag{C.46}$$

$$H^+H^-h_3 : \qquad -\text{Im}(Z_7\,e^{-i\theta_{23}}). \tag{C.47}$$

Likewise, the corresponding $G^+G^-h_k$ interactions are:

$$G^+G^-(c_{12}h_1 + s_{12}h_2) : \qquad Z_1, \tag{C.48}$$

$$G^+G^-(c_{12}h_2 - s_{12}h_1) : \qquad 0, \tag{C.49}$$

$$G^+G^-h_3 : \qquad 0. \tag{C.50}$$

Thus, one can immediately identify $h_1^0 = c_{12}h_1 + s_{12}h_2$, since this linear combination possesses the Higgs couplings of the Standard Model Higgs boson. The second CP-even Higgs state is identified by its non-zero coupling to H^+H^- and depends on whether $Z_7 e^{-i\theta_{23}}$ is purely real or purely imaginary. For example, if $\text{Im}(Z_7 e^{-i\theta_{23}}) = 0$, then $c_{12}h_2 - s_{12}h_1$ is CP-even and h_3 is CP-odd, and vice versa if $\text{Re}(Z_7 e^{-i\theta_{23}}) = 0$.

Cases V$'$ and VI$'$ can be similarly treated. In particular,

$$\text{Case V}' : \quad m_{h_1}^2 = \left[Z_1 + \text{Re}(Z_5 e^{-2i\theta_{23}})\right]v^2, \qquad m_{h_2}^2 = m_{h_3}^2 = Z_1 v^2, \tag{C.51}$$

$$\text{Case VI}' : \quad m_{h_2}^2 = \left[Z_1 + \text{Re}(Z_5 e^{-2i\theta_{23}})\right]v^2, \qquad m_{h_1}^2 = m_{h_3}^2 = Z_1 v^2. \tag{C.52}$$

If we impose the mass ordering $m_{h_1} \leq m_{h_2} \leq m_{h_3}$ in order not to duplicate regions of the 2HDM parameter space, then we can omit Case VI$'$. We summarize the exceptional mass-degenerate cases in Tables XIII, XIV, XV and XVI.

TABLE XIII: Basis-independent conditions for a CP-conserving 2HDM scalar potential and vacuum when $Z_6 = 0$ and Z_5, $Z_7 \neq 0$, assuming at least two degenerate neutral Higgs boson masses. The cases below are exceptional, as they do not arise as limits of Cases I$'$, II$'$ and III$'$ [cf. Table VI]. If we impose the mass-ordering $m_{h_1} \leq m_{h_2} \leq m_{h_3}$, then Cases VI$'$a and b can be eliminated. The neutral Higgs mixing angles θ_{12} in Case IV$'$ and θ_{13} in Cases V$'$ and VI$'$ are defined such that the couplings of h_1^0 (defined as the linear combination of mass-degenerate neutral Higgs fields specified below) coincides precisely with those of the Standard Model Higgs boson. The phase factor η^2 that governs the CP transformation law [cf. eq. (3.7)] is equal to $+1$ in cases IV$'$a, V$'$a, and VI$'$a, and -1 in cases IV$'$b, V$'$b, and VI$'$b. Additional conditions in which Z_7 is replaced by ρ^{Q*} ($Q = U, D$ and E), respectively, must also hold due to the phase correlations implicit in eqs. (3.19) and (3.20). The squared-mass of the two mass-degenerate neutral Higgs states is equal to $Z_1 v^2$, while the third non-degenerate neutral state has a squared-mass equal to $(Z_1 \pm \epsilon_{57}|Z_5|)v^2$, where the plus sign is taken in cases IV$'$b, V$'$a, and VI$'$a, and the minus sign is taken in cases IV$'$a, V$'$b, and VI$'$b.

Cases	conditions [in all cases below, $\text{Im}(Z_5\,e^{-2i\theta_{23}}) = 0$]	A^0	h_1^0	h_2^0
IV$'$a	$s_{13} = \text{Im}(Z_7\,e^{-i\theta_{23}}) = 0$, $Z_1 = Y_2/v^2 + \frac{1}{2}(Z_3 + Z_4 + \epsilon_{57}|Z_5|)$	h_3	$c_{12}h_1 + s_{12}h_2$	$c_{12}h_2 - s_{12}h_1$
IV$'$b	$s_{13} = \text{Re}(Z_7\,e^{-i\theta_{23}}) = 0$, $Z_1 = Y_2/v^2 + \frac{1}{2}(Z_3 + Z_4 - \epsilon_{57}|Z_5|)$	$c_{12}h_2 - s_{12}h_1$	$c_{12}h_1 + s_{12}h_2$	h_3
V$'$a	$c_{12} = \text{Im}(Z_7\,e^{-i\theta_{23}}) = 0$, $Z_1 = Y_2/v^2 + \frac{1}{2}(Z_3 + Z_4 - \epsilon_{57}|Z_5|)$	$c_{13}h_3 + s_{13}h_2$	$c_{13}h_2 - s_{13}h_3$	h_1
V$'$b	$c_{12} = \text{Re}(Z_7\,e^{-i\theta_{23}}) = 0$, $Z_1 = Y_2/v^2 + \frac{1}{2}(Z_3 + Z_4 + \epsilon_{57}|Z_5|)$	h_1	$c_{13}h_2 - s_{13}h_3$	$c_{13}h_3 + s_{13}h_2$
VI$'$a	$s_{12} = \text{Im}(Z_7\,e^{-i\theta_{23}}) = 0$, $Z_1 = Y_2/v^2 + \frac{1}{2}(Z_3 + Z_4 - \epsilon_{57}|Z_5|)$	$c_{13}h_3 - s_{13}h_1$	$c_{13}h_1 + s_{13}h_3$	h_2
VI$'$b	$s_{12} = \text{Re}(Z_7\,e^{-i\theta_{23}}) = 0$, $Z_1 = Y_2/v^2 + \frac{1}{2}(Z_3 + Z_4 + \epsilon_{57}|Z_5|)$	h_2	$c_{13}h_1 + s_{13}h_3$	$c_{13}h_3 - s_{13}h_1$

In the analysis presented above, we assumed that $Z_5 \neq 0$. If $Z_5 = Z_6 = 0$, then eqs. (3.25) and (3.26) imply that h_2^0 and A^0 are mass-degenerate, independently of any special choice for Z_1. In the special case of $Z_1 = Y_2/v^2 + \frac{1}{2}(Z_3 + Z_4)$, all three neutral scalars are degenerate in mass. Moreover, the invariant form of the Higgs squared-mass matrix given

TABLE XIV: The U(2)-invariant quantities $q_{k\ell}$ for Cases IV′a and IV′b

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

TABLE XV: The U(2)-invariant quantities $q_{k\ell}$ for Cases V′a and V′b

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

TABLE XVI: The U(2)-invariant quantities $q_{k\ell}$ for Cases VI′a and VI′b

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

in eq. (2.17) is diagonal. Thus, in this case it is simplest to take $\theta_{12} = \theta_{13} = \theta_{23} = 0$ (instead of imposing a mass ordering of the h_k fields). Eq. (C.21) implies that h_1 is the CP-even neutral Higgs field whose couplings coincide with that of the Standard Model Higgs boson. Eqs. (C.29) and (C.30) imply that h_3 is CP-odd and h_2 is CP-even if $\mathrm{Im}(Z_7 e^{-i\theta_{23}}) = 0$ and vice versa if $\mathrm{Re}(Z_7 e^{-i\theta_{23}}) = 0$. In this case, θ_{23} simply keeps track of the overall phase of Z_7. Finally, in the special case of $Z_5 = Z_6 = Z_7 = 0$ (cf. Section 3.4), the individual CP quantum numbers of h_2 and h_3 can not be determined from the bosonic sector alone.

In Section 4.1.2, we determined the basis-independent conditions for a custodial symmetric scalar potential. In the case of $Z_6 = 0$ and $Z_5, Z_7 \neq 0$, the relevant condition is $Z_4 = \epsilon_{57}|Z_5|$ [cf. eq. (4.46)], which yields $m_{A^0} = m_{H^\pm}$ [cf. eq. (4.49)]. If we apply this limit to Table XIII, we discover that there are two possibilities: either A^0 is degenerate in mass with $H^\pm$ (cases IV′a, V′b and VI′b), or there are two neutral fields, one CP-even and one CP-odd, that are degenerate in mass with $H^\pm$ (cases IV′b, V′a, and VI′a). If $Z_5 \neq 0$, $Z_6 = Z_7 = 0$ and the Higgs–fermion interactions are CP-conserving, then as shown in Section 4.1.3, there are two possible conditions, $Z_4 = \pm\epsilon_{5Q}|Z_5|$, that yield a custodial symmetric scalar potential. Table XIII can again be used if one replaces ε_{57} replaced by ε_{5Q}. As shown in eq. (4.51), the relation $Z_4 = \epsilon_{5Q}|Z_5|$ yields $m_{A^0} = m_{H^\pm}$, and one recovers the results given above for the possible Higgs mass degeneracies. In contrast, the relation $Z_4 = -\epsilon_{5Q}|Z_5|$ yields $m_{H^0} = m_{H^\pm}$. In this case, there are again two possibilities: either H^0 is degenerate in mass with $H^\pm$ (cases IV′b, V′a and VI′a), or there are two neutral CP-even fields, h_1^0 and h_2^0, that are degenerate in mass with $H^\pm$ (cases IV′a, V′b, and VI′b). If one now imposes one additional condition, $Z_4 = Z_5 = 0$, then all three neutral Higgs bosons are degenerate with the charged Higgs boson. Hence, any permutation of possible neutral Higgs mass-degeneracies with the charged Higgs boson is a possible consequence of custodial symmetry, if one allows for sufficiently restrictive conditions on the scalar potential.

Appendix D: Calculation of the 2HDM contributions to S, T and U

The one-loop corrections to the gauge boson two-point functions contain three- and four-point interactions between gauge bosons and the Higgs bosons, the form of which can be read off from eqs. (A.1) and (A.2). The resulting Feynman rules in the t'Hooft-Feynman gauge are exhibited in Table XVII. The 2HDM contributions to S are displayed in Tables XVIII and XIX. The 2HDM contributions to T are displayed in Tables XX and XXI. The 2HDM contributions to U are displayed in Table XXII. The reference Standard Model contributions, which are subtracted out from the 2HDM contributions, are shown in Table XXIII.

The loop integrals are defined and evaluated following ref. [36]:

$$\int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 - m^2)} = \frac{i}{16\pi^2} A_0(m^2), \tag{D.1}$$

$$\int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 - m_1^2)[(k+q)^2 - m_2^2]} = \frac{i}{16\pi^2} B_0(q^2; m_1^2, m_2^2), \tag{D.2}$$

$$\int \frac{d^4k}{(2\pi)^4} \frac{k^\mu k^\nu}{(k^2 - m_1^2)[(k+q)^2 - m_2^2]} = \frac{i}{16\pi^2} g^{\mu\nu} B_{22}(q^2; m_1^2, m_2^2). \tag{D.3}$$
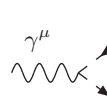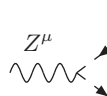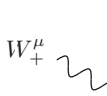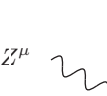
The following two relations are noteworthy:
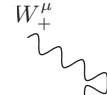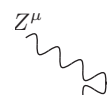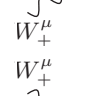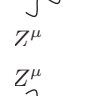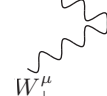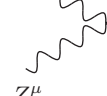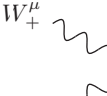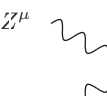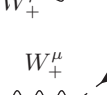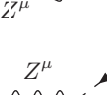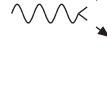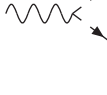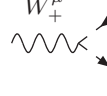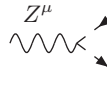
$$B_0(0; m_1^2, m_2^2) = \frac{A_0(m_1^2) - A_0(m_2^2)}{m_1^2 - m_2^2}, \tag{D.4}$$

$$4B_{22}(0; m_1^2, m_2^2) = \mathcal{F}(m_1^2, m_2^2) + A_0(m_1^2) + A_0(m_2^2), \tag{D.5}$$

where

$$\mathcal{F}(m_1^2, m_2^2) \equiv \tfrac{1}{2}(m_1^2 + m_2^2) - \frac{m_1^2 m_2^2}{m_1^2 - m_2^2} \ln\left(\frac{m_1^2}{m_2^2}\right). \tag{D.6}$$

TABLE XVII: Feynman rules used in the calculation of the oblique parameters. The four momentum p_1 points into the vertex, and the four-momentum p_2 points out of the vertex.

W_+^μ, h_k / W_+^μ, h_k	$\frac{1}{2}ig^2 g^{\mu\nu}g^{\mu\nu}$	Z^μ, h_k / Z^μ, h_k	$\frac{ig^2}{2c_W^2}g^{\mu\nu}g^{\mu\nu}$
W_+^μ, H^+ / W_+^μ, H^+	$\frac{1}{2}ig^2 g^{\mu\nu}$	Z^μ, H^+,G^+ / Z^μ, H^+,G^+	$\frac{ig^2}{2c_W^2}(c_W^2-s_W^2)g^{\mu\nu}$
W_+^μ / W_+^μ $\cdots h_k$	$igq_{ik}m_W\, g^{\mu\nu}$	Z^μ / Z^μ $\cdots h_i$	$\frac{ig}{c_W}q_{i1}m_Z\, g^{\mu\nu}$
W_+^μ, H^-, h_k	$-\frac{1}{2}igq_{k2}(p_1+p_2)^\mu$	Z^μ, h_3,G^0, h_2,h_1	$\frac{g}{2c_W}q_{11}(p_1+p_2)^\mu$
W_+^μ, G^-, h_k	$-\frac{1}{2}igq_{k1}(p_1+p_2)^\mu$	Z^μ, h_1,G^0, h_3,h_2	$\frac{g}{2c_W}q_{21}(p_1+p_2)^\mu$
W_+^μ, G^-, ϕ	$-\frac{1}{2}ig(p_1+p_2)^\mu$	Z^μ, h_2,G^0, h_1,h_3	$\frac{g}{2c_W}q_{31}(p_1+p_2)^\mu$
γ^μ, H^+,G^+ / H^+,G^+	$igs_W(p_1+p_2)^\mu$	Z^μ, H^+, H^+	$\frac{ig}{2c_W}(c_W^2-s_W^2)(p_1+p_2)^\mu$
W_+^μ / W_+^μ $\cdots \phi$	$igm_W\, g^{\mu\nu}$	Z^μ / Z^μ $\cdots \phi$	$\frac{ig}{c_W}m_Z\, g^{\mu\nu}$
		Z^μ, ϕ, G^0	$-\frac{g}{2c_W}(p_1+p_2)^\mu$

The contributions to S from the diagrams in Table XVIII, XIX and Table XXIII are evaluated by employing

eq. (5.4) and eq. (5.7), with the following result: [38]

$$S \equiv \frac{16\pi c_W^2}{g^2} \left\{ F_{ZZ}^{2H}(m_Z^2) - F_{ZZ}^{SM}(m_Z^2) - F_{\gamma\gamma}^{2H}(m_Z^2) + F_{\gamma\gamma}^{SM}(m_Z^2) - \frac{c_{2W}}{s_W c_W} \left[F_{Z\gamma}^{2H}(m_Z^2) - F_{Z\gamma}^{SM}(m_Z^2) \right] \right\}$$

$$= \frac{1}{\pi m_Z^2} \left\{ \sum_{k=1}^{3} q_{k1}^2 \left[\mathcal{B}_{22}(m_Z^2; m_Z^2, m_k^2) - m_Z^2 \mathcal{B}_0(m_Z^2; m_Z^2, m_k^2) \right] + q_{11}^2 \mathcal{B}_{22}(m_Z^2; m_2^2, m_3^2) + q_{21}^2 \mathcal{B}_{22}(m_Z^2; m_1^2, m_3^2) \right.$$

$$\left. + q_{31}^2 \mathcal{B}_{22}(m_Z^2; m_1^2, m_2^2) - \mathcal{B}_{22}(m_Z^2; m_{H^\pm}^2, m_{H^\pm}^2) - \mathcal{B}_{22}(m_Z^2; m_Z^2, m_\phi^2) + m_Z^2 \mathcal{B}_0(m_Z^2; m_Z^2, m_\phi^2) \right\},$$

$$(\text{D.7})$$

where the $F_{ij}(m_V^2)$ are defined in eq. (5.4).

TABLE XVIII: Diagrams representing the 2HDM contributions to S, part 1.

The parameter T can be calculated in a similar manner, where eqs. (D.4)–(D.6) are especially useful. Adding the

---

[38] The $2H$ superscript indicates the 2HDM contributions and the SM superscript indicates the contributions from the Standard Model with a reference Higgs mass m_ϕ that is subtracted off from the 2HDM result. This subtraction procedure is necessary in order to get a finite result.

TABLE XIX: Diagrams representing the 2HDM contributions to S, part 2.

Contributions to $\Pi_{\gamma\gamma}^{2H}(m_Z^2)$ and $\Pi_{Z\gamma}^{2H}(m_Z^2)$

contributions to T from all the diagrams shown in Tables XX, XXI and XXIII yields

$$
\alpha T \equiv \frac{A_{WW}^{2H}(0)}{m_W^2} - \frac{A_{ZZ}^{2H}(0)}{m_Z^2} - \left[\frac{A_{WW}^{SM}(0)}{m_W^2} - \frac{A_{ZZ}^{SM}(0)}{m_Z^2} \right]
$$

$$
= \frac{g^2}{16\pi^2 m_W^2} \left\{ \sum_{k=1}^3 |q_{k2}|^2 B_{22}(0; m_{H^\pm}^2, m_k^2) - q_{11}^2 B_{22}(0; m_2^2, m_3^2) - q_{21}^2 B_{22}(0; m_1^2, m_3^2) - q_{31}^2 B_{22}(0; m_1^2, m_2^2) \right.
$$

$$
+ \sum_{k=1}^3 q_{k1}^2 \left[B_{22}(0; m_W^2, m_k^2) - B_{22}(0; m_Z^2, m_k^2) - m_W^2 B_0(0; m_W^2, m_k^2) + m_Z^2 B_0(0; m_Z^2, m_k^2) \right]
$$

$$
\left. - \frac{1}{2} A_0(m_{H^\pm}^2) - B_{22}(0; m_W^2, m_\phi^2) + B_{22}(0; m_Z^2, m_\phi^2) + m_W^2 B_0(0; m_W^2, m_\phi^2) - m_Z^2 B_0(0; m_Z^2, m_\phi^2) \right\},
$$

$$(D.8)$$

where the $A_{ij}(0)$ are defined in eq. (5.4). Using $\alpha = g^2 s_W^2/(4\pi)$ to isolate T and simplifying the result by employing eq. (D.5), we end up with:

$$
T = \frac{1}{16\pi m_W^2 s_W^2} \left\{ \sum_{k=1}^3 |q_{k2}|^2 \mathcal{F}(m_{H^\pm}^2, m_k^2) - q_{11}^2 \mathcal{F}(m_2^2, m_3^2) - q_{21}^2 \mathcal{F}(m_1^2, m_3^2) - q_{31}^2 \mathcal{F}(m_1^2, m_2^2) \right.
$$

$$
+ \sum_{k=1}^3 q_{k1}^2 \left[\mathcal{F}(m_W^2, m_k^2) - \mathcal{F}(m_Z^2, m_k^2) - 4m_W^2 B_0(0; m_W^2, m_k^2) + 4m_Z^2 B_0(0; m_Z^2, m_k^2) \right]
$$

$$
\left. + \mathcal{F}(m_Z^2, m_\phi^2) - \mathcal{F}(m_W^2, m_\phi^2) + 4m_W^2 B_0(0; m_W^2, m_\phi^2) - 4m_Z^2 B_0(0; m_Z^2, m_\phi^2) \right\}.
$$

$$(D.9)$$

TABLE XX: Diagrams representing the 2HDM contributions to T, part 1.
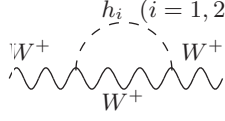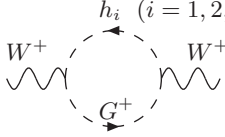
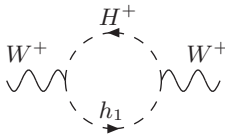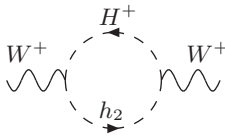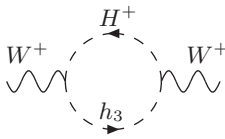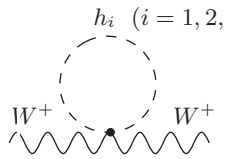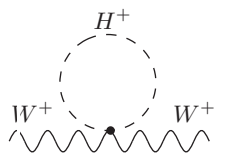| Contributions to $A_{WW}^{2H}(0)$ |
|---|

$$= -\frac{g^2 m_W^2}{16\pi^2} q_{i1}^2 B_0(0; m_W^2, m_i^2)$$

$$= \frac{g^2}{16\pi^2} q_{i1}^2 B_{22}(0; m_W^2, m_i^2)$$

$$= \frac{g^2}{16\pi^2} |q_{12}|^2 B_{22}(0; m_{H^\pm}^2, m_1^2)$$

$$= \frac{g^2}{16\pi^2} |q_{22}|^2 B_{22}(0; m_{H^\pm}^2, m_2^2)$$

$$= \frac{g^2}{16\pi^2} |q_{32}|^2 B_{22}(0; m_{H^\pm}^2, m_3^2)$$

$$= -\frac{1}{2} \frac{g^2}{16\pi^2} A_0(m_i^2)$$

$$= -\frac{1}{2} \frac{g^2}{16\pi^2} A_0(m_{H^\pm}^2)$$

TABLE XXI: Diagrams representing the 2HDM contributions to T, part 2.

Contributions to $A_{ZZ}^{2H}(0)$

$$= -\frac{g^2 m_Z^2}{16\pi^2 c_W^2} q_{i1}^2 B_0(0; m_Z^2, m_i^2)$$

$$= \frac{g^2}{16\pi^2 c_W^2} q_{i1}^2 B_{22}(0; m_Z^2, m_i^2)$$

$$= \frac{g^2}{16\pi^2 c_W^2} q_{21}^2 B_{22}(0; m_1^2, m_3^2)$$

$$= \frac{g^2}{16\pi^2 c_W^2} q_{11}^2 B_{22}(0; m_2^2, m_3^2)$$

$$= \frac{g^2}{16\pi^2 c_W^2} q_{31}^2 B_{22}(0; m_1^2, m_2^2)$$

$$= -\frac{1}{2}\frac{g^2}{16\pi^2 c_W^2} A_0(m_i^2)$$

$$= -\frac{1}{2}\frac{g^2}{16\pi^2 c_W^2} c_{2W}^2 A_0(m_{H^\pm}^2)$$

$$= \frac{g^2}{16\pi^2 c_W^2} c_{2W}^2 B_{22}(0; m_{H^\pm}^2, m_{H^\pm}^2)$$
$$= \frac{1}{2}\frac{g^2}{16\pi^2 c_W^2} c_{2W}^2 A_0(m_{H^\pm}^2)$$

Lastly, adding all of the contributions to $S + U$ in Tables XXII and XXIII gives the following:

$$S + U = \frac{16\pi}{g^2}\left[F_{WW}(m_W^2) - F_{\gamma\gamma}(m_W^2) - \frac{c_W}{s_W} F_{Z\gamma}(m_W^2) \right]$$

$$= \frac{1}{\pi m_W^2}\left\{ -\sum_{k=1}^{3} q_{k1}^2 m_W^2 \mathcal{B}_0(m_W^2; m_W^2, m_k^2) + m_W^2 \mathcal{B}_0(m_W^2; m_W^2, m_\phi^2) - \mathcal{B}_{22}(m_W^2; m_W^2, m_\phi^2) \right.$$

$$\left. + \sum_{k=1}^{3}\left[q_{k1}^2 \mathcal{B}_{22}(m_W^2; m_W^2, m_k^2) + |q_{k2}|^2 \mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_k^2) \right] - 2\mathcal{B}_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2) \right\}. \qquad \text{(D.10)}$$

The formulae for the oblique parameters in a general extended-Higgs sector model with an arbitrary number of scalar singlets and doublets has been presented in ref. [37]. In contrast to our above results, the treatment of ref. [37] employs a basis-dependent scalar-mixing matrix. In particular, our expressions for the oblique parameters depend only on the masses of the physical Higgs fields and the basis-invariant functions $q_{k\ell}$.
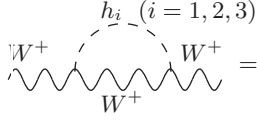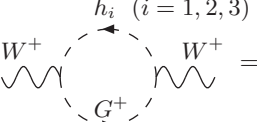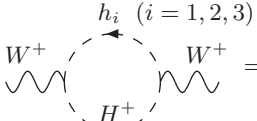
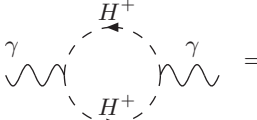TABLE XXII: Diagrams representing the 2HDM contributions to $S + U$.
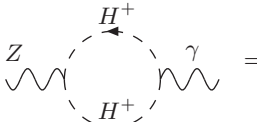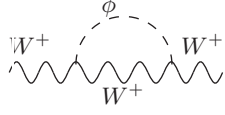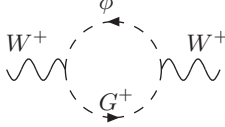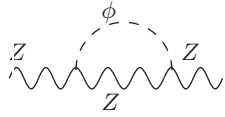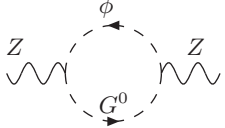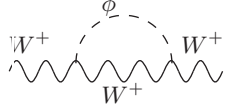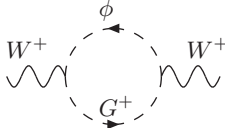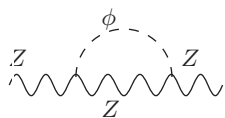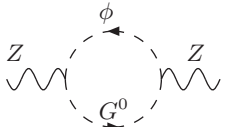
Contributions to $\Pi_{WW}^{2H}(m_W^2)$

$h_i \ (i = 1, 2, 3)$

$W^+ \quad W^+ \quad = -\frac{g^2 m_W^2}{16\pi^2} q_{i1}^2 B_0(m_W^2; m_W^2, m_i^2)$

W^+

$h_i \ (i = 1, 2, 3)$

$W^+ \quad W^+ \quad = \frac{g^2}{16\pi^2} q_{i1}^2 B_{22}(m_W^2; m_W^2, m_i^2)$

G^+

$h_i \ (i = 1, 2, 3)$

$W^+ \quad W^+ \quad = \frac{g^2}{16\pi^2} |q_{i2}|^2 B_{22}(m_W^2; m_{H^\pm}^2, m_i^2)$

H^+

Contributions to $\Pi_{\gamma\gamma}^{2H}(m_W^2)$ and $\Pi_{Z\gamma}^{2H}(m_W^2)$

H^+

$\gamma \quad \gamma \quad = 4\frac{g^2}{16\pi^2} s_W^2 B_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2)$

H^+

H^+

$Z \quad \gamma \quad = 2\frac{g^2 s_W c_{2W}}{16\pi^2 c_W} B_{22}(m_W^2; m_{H^\pm}^2, m_{H^\pm}^2)$

H^+

TABLE XXIII: Standard Model contributions to the oblique parameters.

Contributions to $\Pi_{WW}^{SM}(m_W^2)$ and $\Pi_{ZZ}^{SM}(m_Z^2)$

$$= -\frac{g^2 m_W^2}{16\pi^2} B_0(m_W^2; m_W^2, m_1^2)$$

$$= \frac{g^2}{16\pi^2} B_{22}(m_W^2; m_W^2, m_1^2)$$

$$= -\frac{g^2 m_Z^2}{16\pi^2 c_W^2} B_0(m_Z^2; m_Z^2, m_1^2)$$

$$= \frac{g^2}{16\pi^2 c_W^2} B_{22}(m_Z^2; m_Z^2, m_1^2)$$

Contributions to $A_{WW}^{SM}(0)$ and $A_{ZZ}^{SM}(0)$

$$= -\frac{g^2 m_W^2}{16\pi^2} B_0(0; m_W^2, m_1^2)$$

$$= \frac{g^2}{16\pi^2} B_{22}(0; m_W^2, m_1^2)$$

$$= -\frac{g^2 m_Z^2}{16\pi^2 c_W^2} B_0(0; m_Z^2, m_1^2)$$

$$= \frac{g^2}{16\pi^2 c_W^2} B_{22}(0; m_Z^2, m_1^2)$$

Appendix E: Higgs masses and mixing angles in the decoupling limit

In the decoupling limit of the 2HDM [28], one neutral Higgs boson is kept light, with mass $\lesssim \mathcal{O}(m_Z)$, and the other Higgs boson masses are taken large compared to m_Z. In this case, one can formally integrate out the heavy Higgs states, and the effective low-energy theory consists of a one-Higgs-doublet model. In the decoupling limit, the properties of the light neutral Higgs boson must approach those of the Standard Model Higgs boson. It is simplest to characterize the decoupling limit in the Higgs basis as follows:

$$\text{(i)} \quad |Z_i| \lesssim \mathcal{O}(1) \,, \tag{E.1}$$

$$\text{(ii)} \quad Y_2 \gg v^2 \,. \tag{E.2}$$

We shall define Λ to be the mass scale that characterizes the heavy Higgs states, i.e. $Y_2 \sim \mathcal{O}(\Lambda)$. In light of eq. (2.22), these two requirements imply that $m_{H^\pm} \gg v$.

It is convenient to work in the basis of neutral Higgs mass-eigenstate h_1, h_2 and h_3, in which the corresponding squared-masses are given by eq. (B.3). Assuming eqs. (E.1) and (E.2), the squared-masses are given by:

$$m_1^2 = (s_{12}^2 + c_{12}^2 s_{13}^2) Y_2 + \mathcal{O}(v^2) \,, \tag{E.3}$$

$$m_2^2 = (c_{12}^2 + s_{12}^2 s_{13}^2) Y_2 + \mathcal{O}(v^2) \,, \tag{E.4}$$

$$m_3^2 = c_{13}^2 Y_2 + \mathcal{O}(v^2) \,, \tag{E.5}$$

after employing the q_{k2} given in Table I. In the decoupling limit, precisely two of the three neutral Higgs masses are of $\mathcal{O}(Y_2)$ whereas the third neutral Higgs boson mass is of order $\mathcal{O}(v^2)$. Moreover, to preserve consistency of eqs. (B.5) and (B.6), we required that terms of $\mathcal{O}(Y_2/v^2)$ cancel in these two equations, which yield the conditions:

$$Y_2 s_{13} c_{13} \lesssim \mathcal{O}(v^2) \,, \qquad Y_2 c_{13}^2 s_{12} c_{12} \lesssim \mathcal{O}(v^2) \,. \tag{E.6}$$

The above requirements lead to three possible cases:

$$\textbf{Case I':} \quad |s_{12}| \sim |s_{13}| \lesssim \mathcal{O}(v^2/Y_2) \quad \Longrightarrow \quad m_2, m_3 \gg m_1 \,,$$

$$\textbf{Case II':} \quad |c_{12}| \sim |s_{13}| \lesssim \mathcal{O}(v^2/Y_2) \quad \Longrightarrow \quad m_1, m_3 \gg m_2 \,,$$

$$\textbf{Case III':} \quad |c_{13}| \lesssim \mathcal{O}(v^2/Y_2) \quad \Longrightarrow \quad m_1, m_2 \gg m_3 \,.$$

The nomenclature for these three cases follows that of Appendix C.3, although we do *not* assume that $Z_6 = 0$ in the present discussion. In all three cases, we can now obtain expressions for the corresponding neutral Higgs squared-masses.

In Case I',

$$m_1^2 \simeq Z_1 v^2 \,, \tag{E.7}$$

$$m_2^2 \simeq Y_2 + \tfrac{1}{2}\left[Z_3 + Z_4 + \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) \right] v^2 \,, \tag{E.8}$$

$$m_3^2 \simeq Y_2 + \tfrac{1}{2}\left[Z_3 + Z_4 - \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) \right] v^2 \,. \tag{E.9}$$

In Case II',

$$m_1^2 \simeq Y_2 + \tfrac{1}{2}\left[Z_3 + Z_4 + \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) \right] v^2 \,, \tag{E.10}$$

$$m_2^2 \simeq Z_1 v^2 \,, \tag{E.11}$$

$$m_3^2 \simeq Y_2 + \tfrac{1}{2}\left[Z_3 + Z_4 - \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) \right] v^2 \,. \tag{E.12}$$

In Case III',

$$m_1^2 \simeq Y_2 + \tfrac{1}{2}\left[Z_3 + Z_4 - \mathrm{Re}(Z_5 e^{-2i\overline{\theta}_{23}}) \right] v^2 \,, \tag{E.13}$$

$$m_2^2 \simeq Y_2 + \tfrac{1}{2}\left[Z_3 + Z_4 + \mathrm{Re}(Z_5 e^{-2i\overline{\theta}_{23}}) \right] v^2 \,, \tag{E.14}$$

$$m_3^2 \simeq Z_1 v^2 \,, \tag{E.15}$$

where $\overline{\theta}_{23}$ is defined in eq. (C.20) [cf. the comments that precede this equation]. In all cases above, we omit terms of $\mathcal{O}\left(v^4/Y_2\right)$.

Despite appearances, the above mass formulae are consistent. In Cases I' and II', eq. (B.4) implies that $\text{Im}(Z_5 e^{-2i\theta_{23}}) \lesssim \mathcal{O}\left(v^2/Y_2\right)$. It follows that $\text{Re}(Z_5 e^{-2i\theta_{23}}) = \varepsilon|Z_5| + \mathcal{O}\left(v^2/Y_2\right)$, where

$$\varepsilon \equiv \text{sgn}\left[\text{Re}(Z_5 e^{-2i\theta_{23}})\right].\tag{E.16}$$

Hence, in Cases I' and II', the squared-masses of the two heavy states are given by

$$Y_2 + \tfrac{1}{2}\left(Z_3 + Z_4 \pm |Z_5|\right) + \mathcal{O}\left(\frac{v^2}{Y_2}\right).\tag{E.17}$$

In Case III', eq. (B.6) implies that $\text{Im}(Z_5 e^{-2i\overline{\theta}_{23}}) \lesssim \mathcal{O}\left(v^2/Y_2\right)$. In this case, in then follows that $\text{Re}(Z_5 e^{-2i\overline{\theta}_{23}}) = \overline{\varepsilon}|Z_5| + \mathcal{O}\left(v^2/Y_2\right)$, where $\overline{\varepsilon} = \text{sgn}[\text{Re}(Z_5 e^{-2i\overline{\theta}_{23}})]$. Once again, the squared-masses of the two heavy states again reduce to eq. (E.17).

In the analysis above, no assumption was made for the value of Z_6. If $Z_6 = 0$ then eqs. (C.17)–(C.19) imply that $\text{Im}(Z_5 e^{2i\theta_{23}}) = 0$ in Cases I' and II' and $\text{Im}(Z_5 e^{2i\overline{\theta}_{23}}) = 0$ in Case III'. In this case, one can diagonalize the neutral Higgs squared-mass matrix exactly [cf. eq. (2.17)]. In particular, in the case of $Z_6 = 0$, the squared-mass formulae given in eqs. (E.7)–(E.15) [and in eq. (E.17)] are exact, with no $\mathcal{O}(v^2/Y_2)$ corrections.

In the case of a CP-conserving scalar potential and $Z_6 \neq 0$, we note that Case I of Table II is consistent with Case I' above, and the decoupling limit is specified by $|s_{12}| \sim \mathcal{O}(v^2/Y_2)$. Case IIb of Table II is consistent with Case II' above, and the decoupling limit is specified by $|s_{13}| \sim \mathcal{O}(v^2/Y_2)$. Finally, Case IIa of Table II is consistent with either Cases I' or III'. The corresponding decoupling limit is $|s_{13}| \sim \mathcal{O}(v^2/Y_2)$ in Case I' and $|c_{13}| \sim \mathcal{O}(v^2/Y_2)$ in Case III'.

It is convenient to adopt a convention where $m_1 < m_2, m_3$. In this convention, only Case I' is relevant in the decoupling limit. Henceforth, we shall assume that h_1 is the lightest neutral Higgs boson in the decoupling limit. No mass-ordering of h_2 and h_3, which depends on the sign ε, will be assumed.

For completeness (and as a check of the above results), we provide an alternate derivation of the neutral Higgs squared-masses and mixing in the decoupling limit. We may compute the eigenvalues of eq. (2.17) directly by setting $Z_6 = 0$ and treating Z_6 as a small perturbation. In first approximation,

$$m_1^2 \simeq Z_1 v^2,\tag{E.18}$$
$$m_{2,3}^2 \simeq m_{H^\pm}^2 + \tfrac{1}{2}(Z_4 \pm |Z_5|)v^2,\tag{E.19}$$

where we have used eq. (2.22). To determine which squared masses in eq. (E.19) correspond to h_2 and h_3, one can also treat the off-diagonal 23 and 32 elements of eq. (2.17) perturbatively, in which case one finds:

$$m_2^2 - m_3^2 \simeq \begin{cases} |Z_5|v^2, & \text{for } \text{Re}(Z_5 e^{-2i\theta_{23}}) \geq 0, \\ -|Z_5|v^2, & \text{for } \text{Re}(Z_5 e^{-2i\theta_{23}}) \leq 0. \end{cases}\tag{E.20}$$

That is, all the heavy scalar squared-masses can be written in terms of a single large squared-mass parameter Λ^2 as follows:

$$m_3^2 \equiv \Lambda^2,\tag{E.21}$$
$$m_2^2 = \Lambda^2 + \varepsilon|Z_5|v^2,\tag{E.22}$$
$$m_{H^\pm}^2 = \Lambda^2 - \tfrac{1}{2}\left[Z_4 - \varepsilon|Z_5|\right]v^2,\tag{E.23}$$

where ε is defined in eq. (E.16).

Corrections proportional to Z_6 enter at second-order in perturbation theory and contribute terms that are parametrically smaller than the results displayed in eqs. (E.18) and (E.19). In particular,

$$m_1^2 \simeq Z_1 v^2 - \frac{|Z_6|^2 v^4}{\Lambda^2}.\tag{E.24}$$

The invariant neutral Higgs mixing angles in the decoupling limit can be determined directly from eqs. (C21) and (C25) of ref. [2], which we reproduce below:

$$s_{13}^2 = \frac{(Z_1 v^2 - m_1^2)(Z_1 v^2 - m_2^2) + |Z_6|^2 v^4}{(m_3^2 - m_1^2)(m_3^2 - m_2^2)},\tag{E.25}$$

$$c_{13}^2 s_{12}^2 = \frac{(Z_1 v^2 - m_1^2)(m_3^2 - Z_1 v^2) - |Z_6|^2 v^4}{(m_2^2 - m_1^2)(m_3^2 - m_2^2)}.\tag{E.26}$$

These expressions are exact. Assuming that $Z_5 \neq 0$, it then immediately follows from eqs. (E.21)–(E.24) that:[39]

$$s_{13}^2 \sim s_{12}^2 \sim \mathcal{O}\left(\frac{v^4}{\Lambda^4}\right), \tag{E.27}$$

since the numerators of eqs. (E.25) and (E.26) are of order v^6/Λ^2, whereas the denominators are of order $\Lambda^2 v^2$. Some care is required to treat the case of $Z_5 = 0$ [since in this case $m_2^2 - m_3^2 \lesssim \mathcal{O}(v^4/\Lambda^2)$]. Nevertheless, our original analysis above confirms that eq. (E.27) still holds. Hence, in the decoupling limit,[40]

$$|s_{12}| \sim |s_{13}| \simeq \mathcal{O}\left(\frac{v^2}{\Lambda^2}\right), \qquad c_{12} \sim c_{13} \simeq 1, \tag{E.28}$$

in a convention where h_1 is defined to be the lightest neutral Higgs boson.

In the CP-conserving limit, the neutral Higgs masses in the decoupling limit can be obtained directly from eqs. (3.16) and (3.17) by assuming that $Y_2 \gg Z_1 v^2$. In the case of $Z_6 \neq 0$,

$$m_{h^0}^2 \simeq Z_1 v^2, \tag{E.29}$$
$$m_{H^0}^2 \simeq m_A^2 + \varepsilon_{56}|Z_5|v^2, \tag{E.30}$$
$$m_{A^0}^2 \simeq m_{H^\pm}^2 + \tfrac{1}{2}(Z_4 - \epsilon_{56}|Z_5|)v^2, \tag{E.31}$$

as one approaches the decoupling limit, in agreement with eqs. (E.18) and (E.21)–(E.23). In particular, referring to Table II, we identify $h_1 = h^0$ and

$$h_2 = H^0, \quad h_3 = A^0, \qquad \text{and } \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) = \varepsilon_{56}|Z_5|, \qquad \text{(Case I)} \tag{E.32}$$
$$h_2 = A^0, \quad h_3 = H^0, \qquad \text{and } \mathrm{Re}(Z_5 e^{-2i\theta_{23}}) = -\varepsilon_{56}|Z_5|, \qquad \text{(Case IIa)} \tag{E.33}$$

from which it follows that

$$\varepsilon = \eta^2 \epsilon_{56}. \tag{E.34}$$

In the case of $Z_6 = 0$, eq. (E.29) is an exact result. In addition, eqs. (E.30)–(E.34) apply with ε_{56} replaced by ε_{57} and/or ε_{5Q} as appropriate, with the new versions of eqs. (E.32) and (E.33) applying in Cases I′a and I′b of Table VI, respectively.

Finally, we note that in the limit of custodial symmetry, the 2HDM potential and vacuum are CP-conserving and eq. (4.38) is satisfied. That is,

$$Z_4 = \eta^2 \varepsilon |Z_5|, \tag{E.35}$$

in the case of a generic scalar potential. Consider first the case of $Z_6 \neq 0$. Then, using eqs. (E.29)–(E.31),

$$m_{A^0}^2 - m_{H^\pm}^2 = \tfrac{1}{2}|Z_5|(\eta^2 \varepsilon - \epsilon_{56})v^2, \tag{E.36}$$
$$m_{H^0}^2 - m_{H^\pm}^2 = \tfrac{1}{2}|Z_5|(\eta^2 \varepsilon + \epsilon_{56})v^2. \tag{E.37}$$

Using eq. (E.34), it follows that $m_{H^\pm}^2 = m_{A^0}^2$, as expected. For $Z_6 = 0$ and $Z_7 \neq 0$, simply replace ε_{56} with ε_{57} and the same conclusions follow. In the special case of $Z_6 = Z_7 = 0$ (and assuming CP-conserving Higgs–fermion Yukawa interactions), it is also possible to have a custodial symmetric scalar potential with $Z_4 = -\eta^2 \varepsilon |Z_5|$ [cf. eq. (4.44) and Section 4.1.3]. Replacing ε_{56} above with ε_{5Q}, it then follows that $m_{H^\pm}^2 = m_{H^0}^2$. Of course, both these Higgs mass-degeneracies are enforced by the custodial symmetry independently of the decoupling limit.

Appendix F: Derivation of tree-level unitarity limits

The assumption of tree-level unitarity in scattering processes implies an upper bound on the magnitudes of the Z_i parameters. This places an upper limit on the masses of the heavy Higgs states in parameter regimes in which the

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[39] If $Z_6 = 0$ then $m_1^2 = Z_1 v^2$ is exact, in which case $s_{12} = s_{13} = 0$ with no additional corrections.
[40] By convention, we take $-\tfrac{1}{2}\pi \leq \theta_{12}, \theta_{13} < \tfrac{1}{2}\pi$, in which case $c_{12}, c_{13} \geq 0$.

decoupling limit does not apply. The implications of unitarity for the 2HDM has been studied in the context of the scattering of gauge bosons and the physical scalars in refs. [38, 39]. By placing an upper limit on the amplitude for a process $\varphi_A\varphi_B \to \varphi_C\varphi_D$, one can quantify the constraints from tree-level unitarity as follows:

$$|g_{ABCD}| < 8\pi. \tag{F.1}$$

For tree-level scattering processes, only the quartic bosonic couplings are relevant, namely $W^+W^-W^+W^-$, $W^+W^-H^+H^-$, $(H^+e^{i\theta_{23}})(H^+e^{i\theta_{23}})W^-W^-$ + h.c., $Z^0Z^0Z^0h_m$, $G^0h_mG^-(H^+e^{i\theta_{23}})$ + h.c., $Z^0Z^0H^+H^-$, and $Z^0Z^0W^-(H^+e^{i\theta_{23}})$.

The equivalence theorem [40] allows one equate a high energy scattering amplitude involving gauge bosons to the analogous amplitude involving Goldstone bosons, up to an unimportant overall sign, by making the replacements $W^\pm \to G^\pm$ and $Z^0 \to G^0$. Thus, one can translate limits on the gauge boson/Higgs couplings into limits on the Goldstone/Higgs couplings. The resulting constraints on Z_1, Z_3, $Z_3 + Z_4$, $\mathrm{Re}(Z_5 e^{-2i\theta_{23}})$, and $\mathrm{Re}(Z_6 e^{-i\theta_{23}})$ can be read off directly from eqs. (A.8), as shown in Table XXIV.

TABLE XXIV: Calculation of tree-level unitarity limits on the CP-conserving quartic couplings. Combinatorial factors are included to take into account identical particles.

Relevant term in the scalar potential	Amplitude	Resulting unitarity bound
$\frac{1}{2}Z_1 G^+G^-G^+G^-$	$\frac{1}{16\pi}(\frac{1}{2}Z_1)\cdot 4$	$|Z_1| < 4\pi$
$\frac{1}{2}Z_3 G^0G^0H^+H^-$	$\frac{1}{16\pi}(\frac{1}{2}Z_3)\cdot 2$	$|Z_3| < 8\pi$
$(Z_3+Z_4)G^+G^-H^+H^-$	$\frac{1}{16\pi}(Z_3+Z_4)$	$|Z_3+Z_4| < 8\pi$
$\frac{1}{2}Z_5 e^{-2i\theta_{23}}(H^+e^{i\theta_{23}})(H^+e^{i\theta_{23}})G^-G^-$ + h.c.	$\frac{1}{16\pi}\mathrm{Re}(Z_5 e^{-2i\theta_{23}})\cdot 4$	$|\mathrm{Re}(Z_5 e^{-2i\theta_{23}})| < 2\pi$
$Z_6 e^{-i\theta_{23}}G^0G^0G^-(H^+e^{i\theta_{23}})$ + h.c.	$\frac{1}{16\pi}\mathrm{Re}(Z_6 e^{-i\theta_{23}})\cdot 4$	$|\mathrm{Re}(Z_6 e^{-i\theta_{23}})| < 2\pi$

The CP-violating parameters $\mathrm{Im}(Z_5 e^{-2i\theta_{23}})$ and $\mathrm{Im}(Z_6 e^{-i\theta_{23}})$ appear in a more complicated form in the quartic scalar potential. From the interaction $\frac{1}{2}\mathrm{Im}(q_{m2}Z_6 e^{-i\theta_{23}})G^0G^0G^0h_m$ and Table I, one can write Feynman rules for $m = 1, 2$:

$$g_{G^0G^0G^0h_1} = 3\{-s_{12}\mathrm{Im}[Z_6 e^{-i\theta_{23}}] - c_{12}s_{13}\mathrm{Re}[Z_6 e^{-i\theta_{23}}])\},$$
$$g_{G^0G^0G^0h_2} = 3\{c_{12}\mathrm{Im}[Z_6 e^{-i\theta_{23}}] - s_{12}s_{13}\mathrm{Re}[Z_6 e^{-i\theta_{23}}]\}, \tag{F.2}$$

after including an overall symmetry factor 3! corresponding to three identical particles at the vertex. Unitarity requires $|g_{G^0G^0G^0h_m}| < 8\pi$. It is convenient to combine the two limits in quadrature to isolate $\mathrm{Im}(Z_6 e^{-i\theta_{23}})$. That is, $|g_{G^0G^0G^0h_1}|^2 + |g_{G^0G^0G^0h_2}|^2 < 64\pi^2$, which yields

$$\left[\mathrm{Im}(Z_6 e^{-i\theta_{23}})\right]^2 + s_{13}^2\left[\mathrm{Re}(Z_6 e^{-i\theta_{23}})\right]^2 < \frac{64\pi^2}{9}. \tag{F.3}$$

Since $s_{13}^2\left[\mathrm{Re}(Z_6 e^{-i\theta_{23}})\right]^2$ is real and non-negative, it must be true that $|\mathrm{Im}(Z_6 e^{-i\theta_{23}})| < 8\pi/3$.

Similarly, one can use the term $\frac{1}{2}i\,G^0 h_m\left\{G^-H^+e^{i\theta_{23}}\left[q_{m2}^*Z_4 - q_{m2}Z_5 e^{-2i\theta_{23}}\right] + \text{h.c.}\right\}$ with $m = 1, 2$ to derive

$$g_{G^0G^-(H^+e^{i\theta_{23}})h_1} = -c_{12}s_{13}Z_4 - s_{12}\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) - c_{12}s_{13}\mathrm{Re}(Z_5 e^{-2i\theta_{23}}),$$
$$g_{G^0G^-(H^+e^{i\theta_{23}})h_2} = -s_{12}s_{13}Z_4 + c_{12}\mathrm{Im}(Z_5 e^{-2i\theta_{23}}) - s_{12}s_{13}\mathrm{Re}(Z_5 e^{-2i\theta_{23}}). \tag{F.4}$$

Adding the contributions of the two couplings above in quadrature and applying the unitarity bound yields after some simplification:

$$s_{13}^2\left[Z_4 + \mathrm{Re}(Z_5 e^{-2i\theta_{23}})\right]^2 + \left[\mathrm{Im}(Z_5 e^{-2i\theta_{23}})\right]^2 < 64\pi^2. \tag{F.5}$$

In particular, one must satisfy $|\mathrm{Im}(Z_5 e^{-2i\theta_{23}})| < 8\pi$.

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