

CP violation in 2HDM and EFT: the ZZZ vertex

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ABSTRACT: We study the CP violating ZZZ vertex in the two-Higgs doublet model, which is a probe of a Jarlskog-type invariant in the extended Higgs sector. The form factor f_4^Z is evaluated at one loop in a general R_ξ gauge and its magnitude is estimated in the realistic parameter space. Then we turn to the decoupling limit of the two-Higgs doublet model, where the extra scalars are heavy and the physics can be described by the Standard Model supplemented by higher-dimensional operators. The leading operator contributing to f_4^Z at one loop is identified. The CP violating ZZZ vertex is not generated in the effective theory by dimension-8 operators, but instead arises only at the dimension-12 level, which implies an additional suppression by powers of the heavy Higgs mass scale.

KEYWORDS: Beyond Standard Model, CP violation, Effective Field Theories

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1 Introduction

The LHC experiments announced in 2012 the discovery of a neutral scalar (h) of mass 125 GeV [1, 2], consistent with the 1964 prediction of a Higgs Boson as a by-product of the spontaneous symmetry breaking of a gauge symmetry [3–6]. This opened a very exciting program addressing two fundamental questions: i) how many scalars are there?, and ii) do the couplings of the 125 GeV state conform to the prediction in the Standard Model (SM) of electroweak interactions [7, 8]? Thus far, there is no definite sign of an inconsistency with the SM.

A model independent way to interpret the data is provided by the SM effective field theory (SMEFT), where one allows for all operators constructed from the SM fields, organized in an expansion

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\text{SM}} + \sum_{D=5}^{\infty} \left(\sum_i \frac{c_i^{(D)}}{\Lambda^{D-4}} \mathcal{O}_i^{(D)} \right). \tag{1.1}$$

\mathcal{L}_{SM} is the SM Lagrangian, Λ is the mass scale at which new degrees of freedom become propagating, each $\mathcal{O}_i^{(D)}$ is an $SU(3) \times SU(2) \times U(1)$ invariant operator of dimension D , and $c_i^{(D)}$ the corresponding Wilson coefficient. The new operators modify the interaction

strength of the SM particles, or introduce new interactions that are not predicted within the SM. Identifying their presence in the interaction Lagrangian would not only be an evidence of new physics, but would also give indirect hints about the mass scale and degrees of freedom of the underlying theory beyond the SM.

A complementary approach consists in investigating the constraints that the data place on well motivated theories. One simple example consists in adding one more scalar doublet to the SM. Two Higgs doublet models (2HDMs) are interesting because they contain many properties which one may find in more complicated theories, such as the presence of extra neutral scalars, charged scalars, CP-odd or admixtures of CP-even and CP-odd scalars, the possibilities for spontaneous CP violation or flavour changing neutral scalar interactions, among others [9, 10]. Here we focus on the so-called “complex 2HDM” (C2HDM) [11–18].

2HDMs can be approximated by the SMEFT at energies below the mass scale of the new scalars, where the indirect effects of the new scalars are represented by a tower of the higher-dimensional operators in the Lagrangian. There has been some interest in the matching between the 2HDM parameters and the SMEFT Wilson coefficients [19–25]. This exercise allows one to get some intuition about the pattern of operators expected from realistic extensions of the SM, and to identify the leading new physics effects in a model-independent language. In this paper we discuss how CP violation of the C2HDM is manifested in the SMEFT. More precisely, we concentrate on the CP violating ZZZ vertex, which appears at one loop in the C2HDM. This is an especially interesting observable because it measures directly a Jarlskog-type invariant in the Higgs-gauge sector [26], first introduced in [27, 28]. At the technical level, the C2HDM computation involves loops with both heavy and light particles, which require special care when matching to the low-energy effective theory [29–34]. In fact, we will show that the effective description of the CP violating ZZZ vertex is quite non-trivial in this case. Generally, the lowest order in the SMEFT expansion where the ZZZ vertex may appear is dimension-8 ($\mathcal{O}(\Lambda^{-4})$) [35, 36]. However, it turns out that in the SMEFT matched to the C2HDM at one loop the CP-violating ZZZ vertex is only generated at ($\mathcal{O}(\Lambda^{-8})$), that is by a dimension-12 operator.

Our paper is organized as follows. In section 2 we review the observable form factors associated with the ZZZ vertex. Our C2HDM notation and conventions are summarized in section 3. Section 4 contains the calculation of the CP-violating contribution to the ZZZ vertex in a general R_ξ gauge, which we compare with that in the previous literature [26]. The corresponding calculation and the CP violating operator in the SMEFT is discussed in section 5. Finally, section 6 presents our conclusions. Some technical details concerning approximation of the loop integrals using the method of regions are given in appendix A, while derivation of the CP-violating dimension-12 SMEFT operators using gauge invariant functional methods is given in appendix B.

2 The ZZZ vertex

We start by reviewing the formalism to describe the effective Z^3 vertex [37, 38]. Consider the diagram in figure 1 with two on-shell Z bosons characterized by outgoing 4-momenta p_1 , p_2 and polarization vectors $\epsilon(p_1)$, $\epsilon(p_2)$, and an *off-shell* Z boson with the incoming

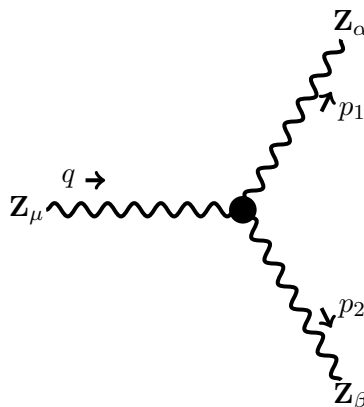


Figure 1. Conventions for the ZZZ vertex $\Gamma_{\mu\alpha\beta}$.

momentum $q = p_1 + p_2$. It follows that $p_1^2 = p_2^2 = m_Z^2$, $p_1 p_2 = q^2/2 - m_Z^2$, $q p_1 = q p_2 = q^2/2$. The blob in figure 1 may represent a contact interaction or particles running in loops. The Lorentz and Bose symmetries constrain the Z^3 vertex function $\Gamma_{\mu\alpha\beta}$ to the following form:

$$\begin{aligned}
 i\Gamma_{\mu\alpha\beta} = & -\frac{q^2 - m_Z^2}{m_Z^2} e f_4^Z(q^2) (\eta_{\mu\alpha} p_{1,\beta} + \eta_{\mu\beta} p_{2,\alpha}) - \frac{q^2 - m_Z^2}{m_Z^2} e f_5^Z(q^2) \epsilon_{\mu\alpha\beta\rho} (p_1 - p_2)^\rho \\
 & + \tilde{f}_1(q^2) (\eta_{\mu\alpha} p_{2,\beta} + \eta_{\mu\beta} p_{1,\alpha}) + \tilde{f}_2(q^2) \eta_{\alpha\beta} q_\mu \\
 & + \tilde{f}_3(q^2) q_\mu p_{1,\beta} p_{2,\alpha} + \tilde{f}_4(q^2) q_\mu p_{1,\alpha} p_{2,\beta} + \tilde{f}_5(q^2) q_\mu (p_{1,\alpha} p_{1,\beta} + p_{2,\alpha} p_{2,\beta}). \tag{2.1}
 \end{aligned}$$

In the first line we have pulled out a function of q^2 from the form factors so as to match the standard notation of ref. [38].¹

The form factor $f_4^Z(q^2)$ corresponds to a C -odd and P -even (thus CP -odd) interaction. One way to see this is to note that an effective Lagrangian with the Z^3 interaction,

$$\mathcal{L}_{\text{eff}} \supset \frac{\tilde{\kappa}_{ZZZ}}{m_Z^2} \partial_\mu Z_\nu \partial^\mu Z^\rho \partial_\rho Z^\nu, \tag{2.2}$$

leads to the tree-level vertex in eq. (2.1) with $f_4^Z(q^2) = \tilde{\kappa}_{ZZZ}$. The CP properties are then easily obtained given C acting as $Z_\mu \rightarrow -Z_\mu$ and P acting as $Z_0 \rightarrow Z_0$, $Z_i \rightarrow -Z_i$, $\partial_0 \rightarrow \partial_0$, $\partial_i \rightarrow -\partial_i$. By similar argument one shows that $f_5^Z(q^2)$ corresponds to a C -odd and P -odd (thus CP -even) interaction.

It is important to stress that the full vertex $\Gamma_{\mu\alpha\beta}$ is not an observable. Nevertheless, the form factors f_4^Z and f_5^Z can be related to observable quantities in the following sense. Consider the amplitude to produce a pair of Z bosons. This process will receive a contribution from the diagram with an intermediate off-shell Z boson in the s-channel: $\mathcal{M}_{f\bar{f}\rightarrow ZZ} = \mathcal{M}_{f\bar{f}\rightarrow ZZ}^{(s)} + \dots$, where the dots stand for other contributions. The s-channel can be written as $\mathcal{M}_{f\bar{f}\rightarrow ZZ}^{(s)} = \frac{1}{q^2 - m_Z^2} \Gamma_{\mu\alpha\beta} \epsilon^\alpha(p_1) \epsilon^\beta(p_2) j^\mu(q)$, where j^μ is the f current to

¹For s-channel production of an on-shell ZZ pair from a conserved current our vertex parametrization in eq. (2.1) and the one in ref. [38] both lead to the same amplitude eq. (2.3). The two parametrizations differ only at the level of non-physical unmeasurable form factors.

which the Z boson couples in the Lagrangian. We assume that j^μ is conserved, $q_\mu j^\mu = 0$, which is the case in the relevant situation of $q\bar{q}$ and e^+e^- collisions in the limit where the fermions are treated as massless. Moreover, $p_1^\alpha \epsilon_\alpha(p_1) = p_2^\beta \epsilon_\beta(p_2) = 0$. Then the s-channel part of the ZZ production amplitude reduces to

$$\mathcal{M}_{f\bar{f}\rightarrow ZZ}^{(s)} = -\frac{1}{m_Z^2} [f_4^Z(q^2) (\eta_{\mu\alpha} p_{1,\beta} + \eta_{\mu\beta} p_{2,\alpha}) + f_5^Z(q^2) \epsilon_{\mu\alpha\beta\rho} (p_1 - p_2)^\rho] \epsilon^\alpha(p_1) \epsilon^\beta(p_2) j^\mu(q). \tag{2.3}$$

As long as it is possible to isolate the s-channel production, the form factors f_4^Z and f_5^Z are measurable. In particular, f_4^Z can be related to experimentally observable CP asymmetries in ZZ production in colliders [26, 39]. On the other hand, the remaining form factors $\tilde{f}_i(q^2)$ in eq. (2.1) are *not* observable; in fact, they may be gauge-dependent in specific calculations.

3 Complex two-Higgs doublet model

In this section we summarize the salient features of the C2HDM, for a review see e.g. [9, 10]. The most general renormalizable scalar potential is

$$\begin{aligned} V = & m_{11}^2 \Phi_1^\dagger \Phi_1 + m_{22}^2 \Phi_2^\dagger \Phi_2 - [m_{12}^2 \Phi_1^\dagger \Phi_2 + \text{h.c.}] \\ & + \frac{1}{2} \lambda_1 (\Phi_1^\dagger \Phi_1)^2 + \frac{1}{2} \lambda_2 (\Phi_2^\dagger \Phi_2)^2 + \lambda_3 (\Phi_1^\dagger \Phi_1) (\Phi_2^\dagger \Phi_2) + \lambda_4 (\Phi_1^\dagger \Phi_2) (\Phi_2^\dagger \Phi_1) \\ & + \left[\frac{1}{2} \lambda_5 (\Phi_1^\dagger \Phi_2)^2 + \lambda_6 (\Phi_1^\dagger \Phi_1) (\Phi_1^\dagger \Phi_2) + \lambda_7 (\Phi_2^\dagger \Phi_2) (\Phi_1^\dagger \Phi_2) + \text{h.c.} \right], \end{aligned} \tag{3.1}$$

where Φ_1 and Φ_2 are complex scalar $SU(2)_L$ doublets, with vacuum expectation values (VEVs) $v_1/\sqrt{2}$ and $v_2/\sqrt{2}$. The parameters m_{11}^2 , m_{22}^2 , and $\lambda_1 \dots \lambda_4$ are real parameters, while m_{12}^2 and $\lambda_5 \dots \lambda_7$ can be complex.

In general, both Φ_1 and Φ_2 can have Yukawa couplings to all the SM fermions. However, this leads to flavour changing neutral scalar interactions (FCNSI), which are tightly constrained by experiment. As a result, it is usually assumed that there is a \mathbb{Z}_2 symmetry [40, 41], acting on the scalars as

$$\Phi_1 \rightarrow \Phi_1, \quad \Phi_2 \rightarrow -\Phi_2, \tag{3.2}$$

with appropriate transformations on the fermions, guaranteeing that fermions of a given charge couple exclusively to one of the two scalar fields.

Of course, one can perform a basis change on the scalar fields. The couplings in the scalar potential and in the Yukawa interactions, as well as the specific implementation of the \mathbb{Z}_2 symmetry, change from one basis to the next; but any physical observable cannot depend on such a choice. We denote by the “ \mathbb{Z}_2 basis”, the basis in which the transformation has the specific form in eq. (3.2). For an exact \mathbb{Z}_2 symmetry, m_{12}^2 , λ_6 , and λ_7 vanish. Since the absence of m_{12}^2 precludes a decoupling limit [42], one usually breaks it softly through $m_{12}^2 \neq 0$. If $\arg(\lambda_5) = 2 \arg(m_{12}^2)$, then we may take both couplings real, and the potential preserves CP. When v_1 and v_2 are also real, there is no CP violation (explicit or spontaneous) and

the model is known as the “real 2HDM”. In contrast, if $\arg(\lambda_5) \neq 2 \arg(m_{12}^2)$, then the potential violates CP explicitly; this is known as the “complex 2HDM” (C2HDM) [11–18]. Here, we will choose a basis where v_1 and v_2 are real, without loss of generality.

It is convenient to introduce the “Higgs basis” [27, 28], defined as the basis where only the first scalar has a VEV. This is obtained through the unitary transformation

$$\begin{pmatrix} H_1 \\ H_2 \end{pmatrix} = \begin{pmatrix} c_\beta & s_\beta \\ -s_\beta & c_\beta \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}, \quad (3.3)$$

where $c_\beta = \cos \beta = v_1/v$, $s_\beta = \sin \beta = v_2/v$, and $v = \sqrt{v_1^2 + v_2^2} = (\sqrt{2}G_F)^{-1/2}$. The doublets in the Higgs basis may be parametrized as

$$H_1 = \begin{pmatrix} -iG^+ \\ \frac{1}{\sqrt{2}}(v + h + iG^0) \end{pmatrix}, \quad H_2 = \begin{pmatrix} H^+ \\ \frac{1}{\sqrt{2}}(R + iI) \end{pmatrix}, \quad (3.4)$$

where G^\pm and G^0 are the Goldstone bosons which, in the unitary gauge, are absorbed as the longitudinal components of W^\pm and Z , while H^\pm are the charged scalars.

The scalar potential in the Higgs basis has the form

$$\begin{aligned} V_H = & Y_1|H_1|^2 + Y_2|H_2|^2 + (Y_3H_1^\dagger H_2 + \text{h.c.}) + \frac{Z_1}{2}|H_1|^4 + \frac{Z_2}{2}|H_2|^4 \\ & + Z_3|H_1|^2|H_2|^2 + Z_4(H_1^\dagger H_2)(H_2^\dagger H_1) \\ & + \left\{ \frac{Z_5}{2}(H_1^\dagger H_2)^2 + (Z_6|H_1|^2 + Z_7|H_2|^2)(H_1^\dagger H_2) + \text{h.c.} \right\}, \end{aligned} \quad (3.5)$$

where we follow the notation of [43]. The parameters $Y_{1,2}$ and $Z_{1,2,3,4}$ are all real; the others are, in general, complex. Note that, in the Higgs basis, H_1 and H_2 are not eigenstates of the \mathbb{Z}_2 symmetry and, therefore, the cross terms proportional to Z_6 and Z_7 are in general present. The stationarity conditions in the Higgs basis read

$$Y_1 = -\frac{Z_1}{2}v^2, \quad Y_3 = -\frac{Z_6}{2}v^2. \quad (3.6)$$

The last equation means that only Z_5 , Z_6 , and Z_7 are independently complex. Thus, all sources of CP violation in the Higgs potential must be related to the invariant quantities $\text{Im}(Z_7Z_6^*)$, $\text{Im}(Z_7^2Z_5^*)$, and $\text{Im}(Z_6^2Z_5^*)$ [27].²

The dictionary between the \mathbb{Z}_2 basis and the Higgs basis for the quadratic terms Y_i is

$$Y_1 = m_{11}^2c_\beta^2 + m_{22}^2s_\beta^2 + 2\text{Re}(m_{12}^2)s_\beta c_\beta, \quad (3.7)$$

$$Y_2 = m_{11}^2s_\beta^2 + m_{22}^2c_\beta^2 - 2\text{Re}(m_{12}^2)s_\beta c_\beta, \quad (3.8)$$

$$Y_3 = (m_{22}^2 - m_{11}^2)s_\beta c_\beta + m_{12}^2c_\beta^2 - m_{12}^{*2}s_\beta^2. \quad (3.9)$$

²If all three invariants are non-vanishing, then only two are independent. But one needs all three in order to cover also the cases in which two invariants vanish but the third does not.

The generated cross-term $H_1^\dagger H_2 + \text{h.c.}$ (coefficient Y_3) can be present even if $m_{12}^2 = 0$, unless $m_{11}^2 = m_{22}^2$ (the masses of Φ_1 and Φ_2 being equal). Similarly, for the quartic terms Z_i :

$$Z_1 = \lambda_1 c_\beta^4 + \lambda_2 s_\beta^4 + 2\lambda_{345} s_\beta^2 c_\beta^2, \quad (3.10)$$

$$Z_2 = \lambda_1 s_\beta^4 + \lambda_2 c_\beta^4 + 2\lambda_{345} s_\beta^2 c_\beta^2, \quad (3.11)$$

$$Z_{i=3,4} = (\lambda_1 + \lambda_2 - 2\lambda_{345}) s_\beta^2 c_\beta^2 + \lambda_i, \quad (3.12)$$

$$Z_5 = (\lambda_1 + \lambda_2 - 2\lambda_{345}) s_\beta^2 c_\beta^2 + \lambda_5 c_\beta^2 + \lambda_5^* s_\beta^2, \quad (3.13)$$

$$Z_6 = -s_\beta c_\beta [\lambda_1 c_\beta^2 - \lambda_2 s_\beta^2 - \lambda_{345} c_{2\beta} - i\text{Im}(\lambda_5)], \quad (3.14)$$

$$Z_7 = -s_\beta c_\beta [\lambda_1 s_\beta^2 - \lambda_2 c_\beta^2 + \lambda_{345} c_{2\beta} + i\text{Im}(\lambda_5)], \quad (3.15)$$

where $\lambda_{345} = \lambda_3 + \lambda_4 + \text{Re}(\lambda_5)$. What is relevant is that not all Z_i are independent, as they satisfy the relations:

$$\begin{aligned} Z_2 - Z_1 &= \frac{1 - 2s_\beta^2}{s_\beta c_\beta} \text{Re}(Z_6 + Z_7), \\ Z_{345} - Z_1 &= \frac{1 - 2s_\beta^2}{s_\beta c_\beta} \text{Re}(Z_6) - \frac{2s_\beta c_\beta}{1 - 2s_\beta^2} \text{Re}(Z_6 - Z_7), \end{aligned} \quad (3.16)$$

$$\text{Im}(Z_6 + Z_7) = 0,$$

$$\text{Im}(Z_6 - Z_7) = \frac{2c_\beta s_\beta}{1 - 2s_\beta^2} \text{Im}(Z_5),$$

where $Z_{345} \equiv Z_3 + Z_4 + \text{Re}(Z_5)$, and the first two equations are those relevant for the real 2HDM discussed in [43]. Using these relations we can eliminate for example Z_6 and Z_7 , and express our results in terms of the remaining Z_i . Thus, in the C2HDM, all CP violation invariants in the Higgs potential are proportional to a single phase, which comes from $\text{Im}(m_{12}^2 \lambda_5^*)$ in the original basis.

One goes from the neutral scalars $\{h, R, I\}$ written in the Higgs basis into the neutral scalar mass basis $\{h_1, h_2, h_3\}$ through [18]

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = T^T \begin{pmatrix} h \\ R \\ I \end{pmatrix}, \quad (3.17)$$

where

$$T^T = \begin{pmatrix} \tilde{c}_1 c_2 & \tilde{s}_1 c_2 & s_2 \\ -(\tilde{c}_1 s_2 s_3 + \tilde{s}_1 c_3) & \tilde{c}_1 c_3 - \tilde{s}_1 s_2 s_3 & c_2 s_3 \\ -\tilde{c}_1 s_2 c_3 + \tilde{s}_1 s_3 & -(\tilde{c}_1 s_3 + \tilde{s}_1 s_2 c_3) & c_2 c_3 \end{pmatrix} \quad (3.18)$$

and $s_i = \sin \alpha_i$ and $c_i = \cos \alpha_i$ ($i = 2, 3$). Similarly, $\tilde{s}_1 = \sin \tilde{\alpha}_1$ and $\tilde{c}_1 = \cos \tilde{\alpha}_1$, where $\tilde{\alpha}_1 = \alpha_1 - \beta$. We have defined T to agree with the definition in ref. [10]. In the C2HDM one usually defines a matrix R such that

$$T^T = RR_H = \begin{pmatrix} c_1 c_2 & s_1 c_2 & s_2 \\ -(c_1 s_2 s_3 + s_1 c_3) & c_1 c_3 - s_1 s_2 s_3 & c_2 s_3 \\ -c_1 s_2 c_3 + s_1 s_3 & -(c_1 s_3 + s_1 s_2 c_3) & c_2 c_3 \end{pmatrix} \begin{pmatrix} c_\beta - s_\beta & 0 \\ s_\beta & c_\beta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (3.19)$$

The angles α_1 , α_2 , and α_3 were introduced in [13], and, without loss of generality, may be restricted to

$$-\pi/2 < \alpha_1 \leq \pi/2, \quad -\pi/2 < \alpha_2 \leq \pi/2, \quad 0 \leq \alpha_3 \leq \pi/2. \quad (3.20)$$

The real 2HDM may be obtained by setting $s_2 = s_3 = 0$, and the usual $\alpha = \alpha_1 - \pi/2$.

In the Higgs basis h is the only scalar field that has a coupling to two gauge bosons, and it coincides with the SM one g_{hVV}^{SM} . Thus,

$$g_{h_k VV} = g_{hVV}^{\text{SM}} T_{1k}. \quad (3.21)$$

In the C2HDM,

$$T_{1k} = c_\beta R_{k1} + s_\beta R_{k2}, \quad (3.22)$$

and the coupling of the lightest Higgs to gauge bosons is given by

$$g_{h_1 VV} = g_{hVV}^{\text{SM}} c_2 \cos(\alpha_1 - \beta), \quad (3.23)$$

which reduces in the real 2HDM to $g_{h_1 VV} = g_{hVV}^{\text{SM}} \sin(\beta - \alpha)$. Notice that, since the matrix T is orthogonal, eq. (3.21) implies that

$$\sum_k |g_{h_k VV}|^2 = |g_{hVV}^{\text{SM}}|^2 \quad (3.24)$$

and the coupling of each scalar mass eigenstate with two vector bosons must be smaller than the corresponding coupling in the SM. This property generalizes to any multi Higgs doublet model, so that a value well above the SM would exclude the SM and also all such models. Conversely, since the measurements are consistent with a coupling of the 125 GeV scalar with two gauge bosons very close to the SM value, then the mixing angles in T must be such that this scalar almost coincides with the h in the Higgs basis. This translates into the so-called *alignment limit* of

$$s_2 \rightarrow 0 \quad \text{and} \quad \sin(\alpha_1 - \beta) \rightarrow 0 \quad (\text{C2HDM}), \quad (3.25)$$

and

$$\cos(\beta - \alpha) \rightarrow 0 \quad (\text{real 2HDM}), \quad (3.26)$$

in the C2HDM and real 2HDM, respectively.

4 CP-violating ZZZ vertex in C2HDM

We turn to the calculation of one-loop contributions to the ZZZ vertex in the C2HDM. The goal is to determine the CP-violating form factor $f_4^Z(q^2)$ defined by eq. (2.1) (the other physical form factor $f_5^Z(q^2)$ vanishes at one loop). To that end, we can neglect all the Lorentz structures that are not of the form $\eta^{\mu\alpha} p_1^\beta$ or $\eta^{\mu\beta} p_2^\alpha$. A good consistency check is to verify that these two Lorentz structures have the same coefficient, as the result should be invariant for the exchange $(p_1, \alpha) \leftrightarrow (p_2, \beta)$. We perform the calculation in a general R_ξ gauge, and verify gauge invariance at the end of the calculation. We express the results in terms of the Passarino-Veltman (PV) functions [44], following the LoopTools conventions [45]. To evaluate the loop integrals we use the Mathematica packages FeynCalc [46], and we cross-checked the result with Package-X [47]. Our final result disagrees with the previous literature [26], therefore we will present in some detail the intermediate steps of our calculation.

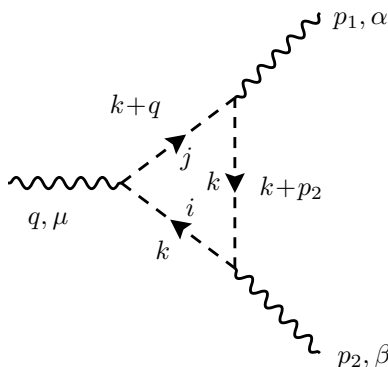


Figure 2. Contribution to the Z^3 vertex $\Gamma_{\mu\alpha\beta}$ with three Higgs h_i, h_j, h_k in the loop.

4.1 Couplings and propagators

For our calculation, we need the following vertices [48],

$$[h_i, h_j, Z^\mu] = \frac{g}{2c_W} (p_i - p_j)^\mu \epsilon_{ijk} x_k, \tag{4.1}$$

$$[Z^\mu, G^0, h_i] = \frac{g}{2c_W} (p_i - p_0)^\mu x_i, \tag{4.2}$$

$$[h_i, Z^\mu, Z^\nu] = i \frac{g}{c_W} m_Z g^{\mu\nu} x_i, \tag{4.3}$$

where $c_W = \cos \theta_W$, all momenta are incoming, and the i of the Feynman rules is already included.³ The coefficient x_i above is related to the C2HDM parameters as

$$x_i \equiv T_{1i} = [c_\beta R_{i1} + s_\beta R_{i2}]. \tag{4.4}$$

That is, x_i coincide with the T_{1i} in eq. (3.22). As we are doing the calculation in a general R_ξ gauge, we also need the propagators for the Goldstone G^0 and the Z in this gauge [49],

$$[G^0, G^0] = \frac{i}{p^2 - \xi m_Z^2 + i\epsilon}, \tag{4.5}$$

$$[Z^\mu, Z^\nu] = -i \frac{1}{k^2 - m_Z^2 + i\epsilon} \left[g^{\mu\nu} - (1 - \xi) \frac{k^\mu k^\nu}{k^2 - \xi m_Z^2} \right]. \tag{4.6}$$

4.2 Diagrams with h_i, h_j, h_k

We start with the diagrams containing only Higgs bosons in the internal lines, as shown in figure 2. Because of the coupling structure in eq. (4.1), all the three scalars have to be different. We get the same result as in ref. [26],

$$e \frac{q^2 - m_Z^2}{m_Z^2} f_4^{Z, hhh} = -\frac{8}{16\pi^2} \left(\frac{g}{2c_W} \right)^3 x_1 x_2 x_3 \sum_{i,j,k} \epsilon_{ijk} C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_j^2, m_k^2). \tag{4.7}$$

³Note that we use the convention for the gauge couplings where the covariant derivatives are written as $D_\mu = \partial_\mu + igA_\mu$. If the opposite convention ($D_\mu = \partial_\mu - igA_\mu$) were used, then the sign of the vertices $[h_i, h_j, Z^\mu]$ and $[Z^\mu, G^0, h_i]$ would be flipped and the Z^3 form factor calculated below would pick up an overall minus sign. When the form factor is included for example into the $f\bar{f} \rightarrow Z^* \rightarrow ZZ$ amplitude, this sign cancels with the corresponding sign choice for the $[f, \bar{f}, Z]$ vertex; only the product $[f, \bar{f}, Z] f_4^Z$ has physical meaning.

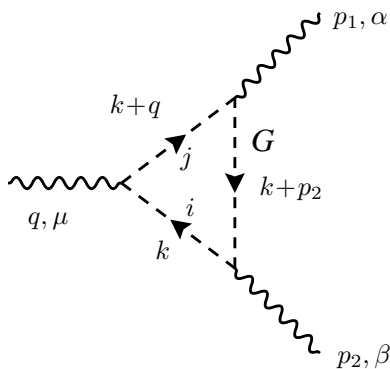


Figure 3. Contribution to the Z^3 vertex $\Gamma_{\mu\alpha\beta}$ with h_i, h_j, G^0 in the loop.

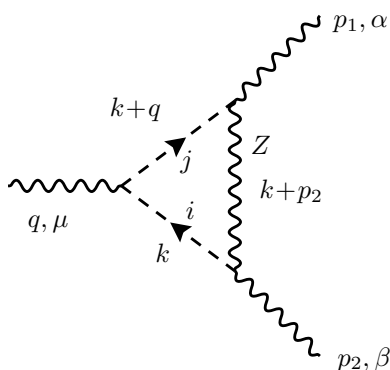


Figure 4. Contribution to the Z^3 vertex $\Gamma_{\mu\alpha\beta}$ with h_i, h_j, Z^0 in the loop.

4.3 Diagrams with h_i, h_j, G^0

We consider now the diagram with one Goldstone boson in one of the internal lines (there are no diagrams with either two or three Goldstone bosons), as shown in figure 3. There are two more diagrams with the G^0 in the other internal lines. Each of them will have all the possible combinations of h_i, h_j . As before, due to the coupling structure in eq. (4.1) and eq. (4.2), we must have $i \neq j$ in all possible combinations. In the R_ξ gauge, we get the result,

$$e \frac{q^2 - m_Z^2}{m_Z^2} f_4^{Z, hhG} = \frac{8}{16\pi^2} \left(\frac{g}{2c_W} \right)^3 x_1 x_2 x_3 \sum_{i,j,k} \epsilon_{ijk} [C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_j^2, \xi m_Z^2) \quad (4.8)$$

$$+ C_{001}(q^2, m_Z^2, m_Z^2, \xi m_Z^2, m_j^2, m_k^2) + C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, \xi m_Z^2, m_k^2)],$$

which agrees with ref. [26] in the Feynman gauge limit $\xi = 1$.

4.4 Diagrams with h_i, h_j, Z

Finally, we evaluate the contribution from the diagrams with one Z boson in an internal line (again there are no diagrams with two or three Z bosons in internal lines), as shown

in figure 4. We get

$$\begin{aligned}
 e \frac{q^2 - m_Z^2}{m_Z^2} f_4^{Z, hhZ} &= \frac{8}{16\pi^2} \left(\frac{g}{2c_W} \right)^3 x_1 x_2 x_3 \sum_{i,j,k} \epsilon_{ijk} [C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_j^2, m_Z^2) \quad (4.9) \\
 &+ C_{001}(q^2, m_Z^2, m_Z^2, m_j^2, m_k^2) + C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_Z^2, m_k^2)] \\
 &- \frac{8}{16\pi^2} \left(\frac{g}{2c_W} \right)^3 x_1 x_2 x_3 \sum_{i,j,k} \epsilon_{ijk} [C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_j^2, \xi m_Z^2) \\
 &+ C_{001}(q^2, m_Z^2, m_Z^2, \xi m_Z^2, m_j^2, m_k^2) + C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, \xi m_Z^2, m_k^2)] \\
 &- \frac{8}{16\pi^2} \left(\frac{g}{2c_W} \right)^3 x_1 x_2 x_3 m_Z^2 \sum_{i,j,k} \epsilon_{ijk} C_1(q^2, m_Z^2, m_Z^2, m_i^2, m_Z^2, m_k^2).
 \end{aligned}$$

In the limit $\xi = 1$ this result differs in the overall sign from that in ref. [26].

4.5 Final result

Summing the different contributions, $f_4^Z = f_4^{Z, hhh} + f_4^{Z, hhZ} + f_4^{Z, hhG}$, we find that the ξ dependent parts of eqs. (4.8) and (4.9) cancel out, ensuring gauge invariance of the final result. Also the antisymmetry of each term in eqs. (4.7), (4.8) and (4.9) implies that the divergences originating from the PV function C_{001} cancel and the final result is finite. All in all, the CP violating Z^3 form factor expressed by the PV functions takes the form

$$\begin{aligned}
 e \frac{q^2 - m_Z^2}{m_Z^2} f_4(q^2) \left[\frac{1}{16\pi^2} \left(\frac{g}{c_W} \right)^3 x_1 x_2 x_3 \right]^{-1} &\equiv \hat{f}_4^Z = \\
 &= \sum_{i,j,k} \epsilon_{ijk} [-C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_j^2, m_k^2) + C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_j^2, m_Z^2) \\
 &+ C_{001}(q^2, m_Z^2, m_Z^2, m_j^2, m_k^2) + C_{001}(q^2, m_Z^2, m_Z^2, m_i^2, m_Z^2, m_k^2) \\
 &- m_Z^2 C_1(q^2, m_Z^2, m_Z^2, m_i^2, m_Z^2, m_k^2)]. \quad (4.10)
 \end{aligned}$$

The dependence of the form factor on q^2 is illustrated in figure 5 for several choices of the heavy scalar spectrum. The order of magnitude of $|f_4^Z|$ that can be achieved in the realistic parameter space of the C2HDM is shown in figure 6, reaching the values of order 10^{-5} . For comparison, the recent ATLAS [50] and CMS [51] analyses of ZZ production at the LHC set upper bounds on $|f_4^Z|$ (assumed real) on the order of 10^{-3} . When considering a generic framework beyond the SM, one must check whether effects other than f_4^Z may contribute to the actual experimental observable being measured (and from which f_4^Z is inferred). For example, one can see from figure 1 in ref. [51] that there is a contribution from $h_{125} \rightarrow ZZ$ to the four lepton events from which f_4^Z is extracted. For the SM Higgs this is not a problem, since this is merely an order 5% contribution to the cross section and, moreover, the measurement of f_4^Z is made by requiring in addition that each Z in the final state has a mass in the range 60-120 GeV. But it could be a concern if a heavier Higgs were to decay into ZZ , competing with the signal from the ZZZ vertex. This problem is mitigated in the C2HDM because of a combination of two facts. First, we know from the $h_{125} \rightarrow ZZ$ measurements that the corresponding coupling in the C2HDM lies very close to

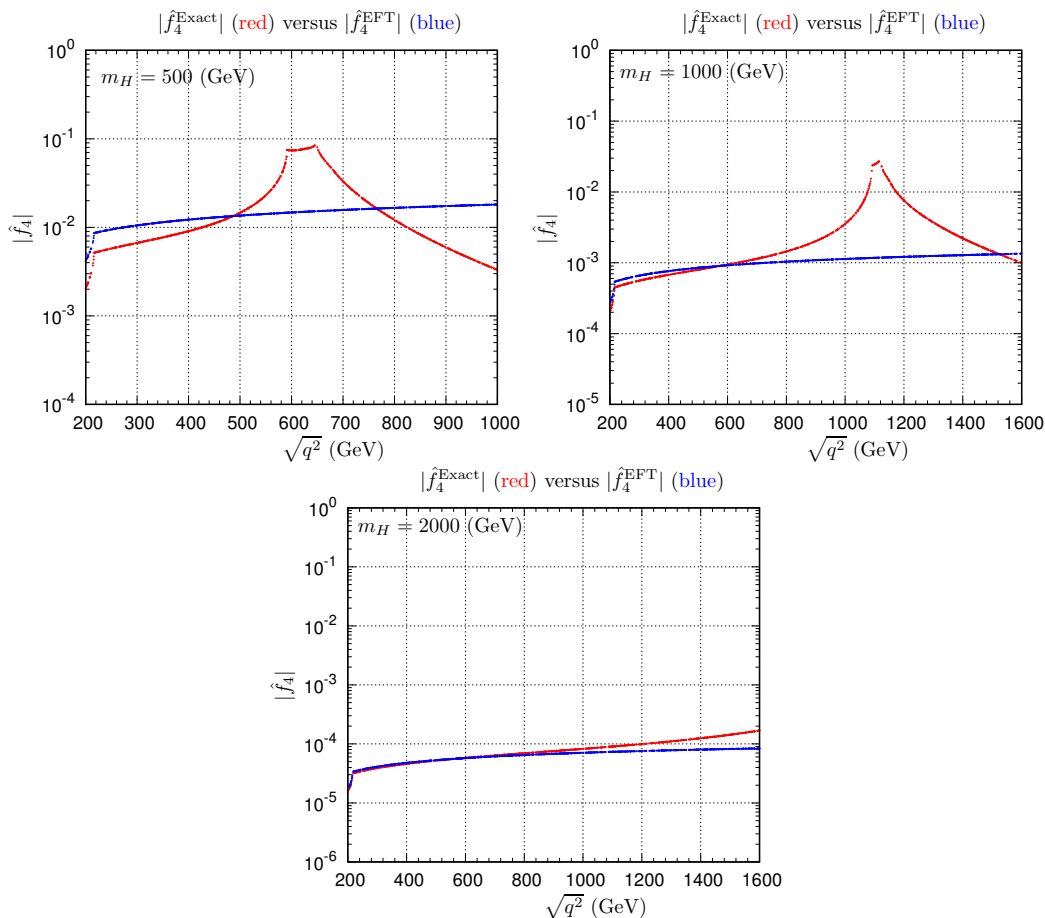


Figure 5. Red: the normalized form factor $\hat{f}_4^Z(q^2)$ as defined in eq. (4.10). We show the dependence on $\sqrt{q^2}$ for 3 different values m_H of the second neutral Higgs mass. The heaviest neutral Higgs mass is assumed to be $\sqrt{m_H^2 + v^2}$. Blue: the same observable calculated in the matched SMEFT (cf. eq. (5.1) in section 5).

the SM value (the so-called alignment limit). Second, the sum rule in eq. (3.24) guarantees that any heavier scalar will have a very small coupling to ZZ . Nevertheless, once statistics improve at LHC, a precise constraint on f_4^Z can best be achieved by a detailed simulation of the C2HDM within the experimental analysis of the collaborations, which is beyond the scope of this work. Our results for the maximum of $|f_4^Z|$ are slightly below those reported in ref. [26]. This is mainly due to the effect of including in our scan the bound on the electron EDM [52]. The sign difference that we have found does not affect much the absolute value, because the diagram where it occurs is typically the dominant one (in the gauge $\xi = 1$) [26].

For future reference, we also give the final form of the Z^3 vertex before evaluating the loop integrals:

$$i\Gamma_{\mu\alpha\beta} = -i \left(\frac{g}{c_W} \right)^3 (x_1 x_2 x_3) \int \frac{d^4 k}{(2\pi)^4} \epsilon_{ijk} \left\{ \frac{k_\mu k_\alpha k_\beta}{((k-p_1)^2 - m_i^2)((k+p_2)^2 - m_j^2)(k^2 - m_k^2)} \right. \\ \left. - \frac{k_\mu k_\alpha k_\beta}{((k-p_1)^2 - m_j^2)((k+p_2)^2 - m_k^2)(k^2 - m_Z^2)} \right.$$

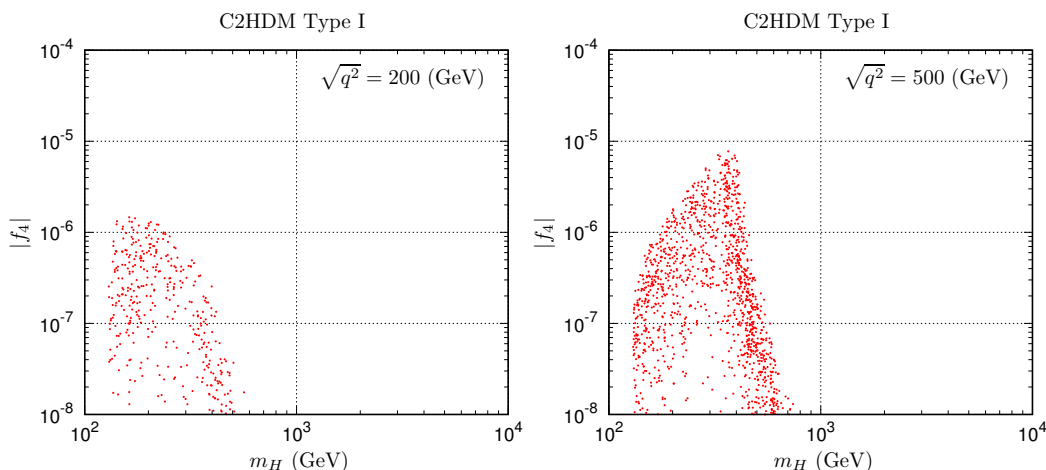


Figure 6. Scatter plots showing the absolute value of the CP violating form factor $f_4^Z(q^2)$ for two values of $\sqrt{q^2}$ for points in the parameter space of the type-1 C2HDM satisfying theoretical (unitarity, bounded from below) and experimental (LHC Higgs, electric dipole moments, and electroweak precision measurements) constraints.

$$\begin{aligned}
 & - \frac{k_\mu k_\alpha k_\beta}{((k-p_1)^2 - m_Z^2)((k+p_2)^2 - m_j^2)(k^2 - m_k^2)} \\
 & - \frac{k_\mu k_\alpha k_\beta}{((k-p_1)^2 - m_k^2)((k+p_2)^2 - m_Z^2)(k^2 - m_j^2)} \\
 & + \frac{m_Z^2 k_\beta \eta_{\mu\alpha}}{((k-p_1)^2 - m_Z^2)((k+p_2)^2 - m_j^2)(k^2 - m_k^2)} \\
 & - \frac{m_Z^2 k_\alpha \eta_{\mu\beta}}{((k-p_1)^2 - m_j^2)((k+p_2)^2 - m_Z^2)(k^2 - m_k^2)} \Bigg\} + (\text{ILS}), \quad (4.11)
 \end{aligned}$$

where ILS stands for (in general divergent and gauge dependent) irrelevant Lorentz structures that do not contribute to the observable form factors. In this form the vertex is manifestly symmetric under interchanging $p_1 \leftrightarrow p_2$, $\alpha \leftrightarrow \beta$. Performing the momentum integral and extracting from the coefficient of the tensor structure $\eta_{\mu\alpha} p_{1,\beta} + \eta_{\mu\beta} p_{2,\alpha}$, cf. eq. (2.1), one obtains the result in eq. (4.10).

5 CP-violating ZZZ vertex in SMEFT

In this section we discuss how the CP-violating ZZZ vertex arises in the low-energy EFT where the heavy non-SM scalars of the C2HDM are integrated out. We denote $m_1 = m_h = 125$ GeV, $m_2 = m_H$, $m_3 = \sqrt{m_H^2 + \delta^2}$ with $\delta \sim v$, and we are interested in the decoupling limit $m_H \gg m_h$. In such a case, only the SM degrees of freedom are available at the energies $E \sim v \ll m_H$. In this regime the dynamics is described by the SMEFT, with the SM Lagrangian augmented by higher-dimensional operators. At the level of dimension-6 operators the matching of the SMEFT Lagrangian to the 2HDM UV completion was discussed e.g. in refs. [19–21, 23, 25, 53, 54]. However, within the EFT framework studied in these references,

there is no source of CP violation contributing to the ZZZ vertex. Below we will identify the higher-dimensional CP-violating operator and discuss how the ZZZ vertex is generated.

The first step toward this goal is to expand the form factor $f_4^Z(q^2)$ in powers of $1/m_H$. In principle, one could expand the result in eq. (4.9) using the known expressions for the PV functions. In practice, this path is difficult due to a complicated form and non-analytic behavior of the PV functions involved. Instead, we find it easier to apply the method of regions [55]. A loop integral containing two disparate mass scales $m_{\text{light}} \ll m_{\text{heavy}}$ can be calculated by A) expanding the integrand for $k \sim m_{\text{light}}$ and performing the integral, B) expanding the integrand for $k \sim m_{\text{heavy}}$ and performing the integral, and then adding these two contributions together. An important point here is that both A) and B) have a clear counterpart on the EFT side where the scales m_{heavy} are integrated out. Namely, A) corresponds to *1-loop* Feynman diagrams with the light particles in the loop and an insertion of tree-level-generated effective operators, while B) corresponds to *tree-level* diagrams with an insertion of operators whose Wilson coefficients are suppressed by a loop factor. Applying the method of regions to the integrals in eq. (4.11) we find that the leading contributions to the sum of the integrals are $\mathcal{O}(m_H^{-4})$ and come from the diagrams with one heavy scalar and two SM particles in the loop (h , Z , or the corresponding Goldstone boson). Moreover, we find that it is the soft region A), $k \ll m_H$, which dominates. Other diagrams and integration regions contribute only at $\mathcal{O}(m_H^{-6})$ or higher. This immediately tells us that, in the EFT for the 2HDM, the CP-violating ZZZ vertex is generated at one loop via diagrams with h , Z in the loop and an insertion of a tree-level-generated effective operator.

In appendix A we give the details of the method of regions applied to eq. (4.11), albeit for the sake of brevity we work there in the simplified limit $m_h \rightarrow m_Z$. Here we write down the leading contribution to the CP-violating form factor f_4^Z for a general m_h , valid for $m_h \ll m_H$ and $q^2 \ll m_H^2$:

$$\begin{aligned}
 e f_4^Z(q^2) \approx & \frac{\delta^2 x_1 x_2 x_3}{m_H^4} \left(\frac{g}{c_W} \right)^3 \frac{1}{384 \pi^2 m_Z^4 q^6 (q^2 - m_Z^2)} \left\{ \right. \\
 & + 2 m_h^2 m_Z^2 q^6 (m_h^4 - 5 m_h^2 m_Z^2 + 10 m_Z^4) \text{DiscB}(m_Z^2, m_h, m_Z) \\
 & - 2 m_Z^6 q^2 \text{DiscB}(q^2, m_h, m_Z) \times \\
 & \times [m_h^6 - m_h^4 (3 m_Z^2 + 2 q^2) + m_h^2 (3 m_Z^4 + 6 m_Z^2 q^2 + q^4) - m_Z^2 (m_h^4 + 4 m_Z^2 q^2 - 5 q^4)] \\
 & + m_Z^2 q^2 (m_Z^2 - m_h^2) (m_Z^2 - q^2) (2 m_h^4 (m_Z^2 + q^2) - m_h^2 (4 m_Z^4 + 9 m_Z^2 q^2) + 2 m_Z^6 + 9 m_Z^4 q^2) \\
 & + [m_h^8 (m_Z^4 + m_Z^2 q^2 + q^4) - m_h^6 (4 m_Z^6 + 7 m_Z^4 q^2 + 7 m_Z^2 q^4) + 3 m_h^4 (2 m_Z^8 + 5 m_Z^6 q^2 + 6 m_Z^4 q^4) \\
 & \left. - m_h^2 m_Z^6 (4 m_Z^4 + 13 m_Z^2 q^2 + 13 q^4) + m_Z^8 (m_Z^4 + 4 m_Z^2 q^2 - 5 q^4)] (m_Z^2 - q^2) \log \left(\frac{m_h^2}{m_Z^2} \right) \right\}, \tag{5.1}
 \end{aligned}$$

where we introduced the DiscB function as defined in [47]:

$$\begin{aligned}
 \text{DiscB}(p^2, m_1, m_2) &= \lambda(p^2, m_1, m_2) \log \left(\frac{m_1^2 + m_2^2 - p^2 + p^2 \lambda(p^2, m_1, m_2)}{2 m_1 m_2} \right), \\
 \lambda(p^2, m_1, m_2) &= \sqrt{1 - \frac{2(m_1^2 + m_2^2)}{p^2} + \frac{(m_1^2 - m_2^2)^2}{p^4}}. \tag{5.2}
 \end{aligned}$$

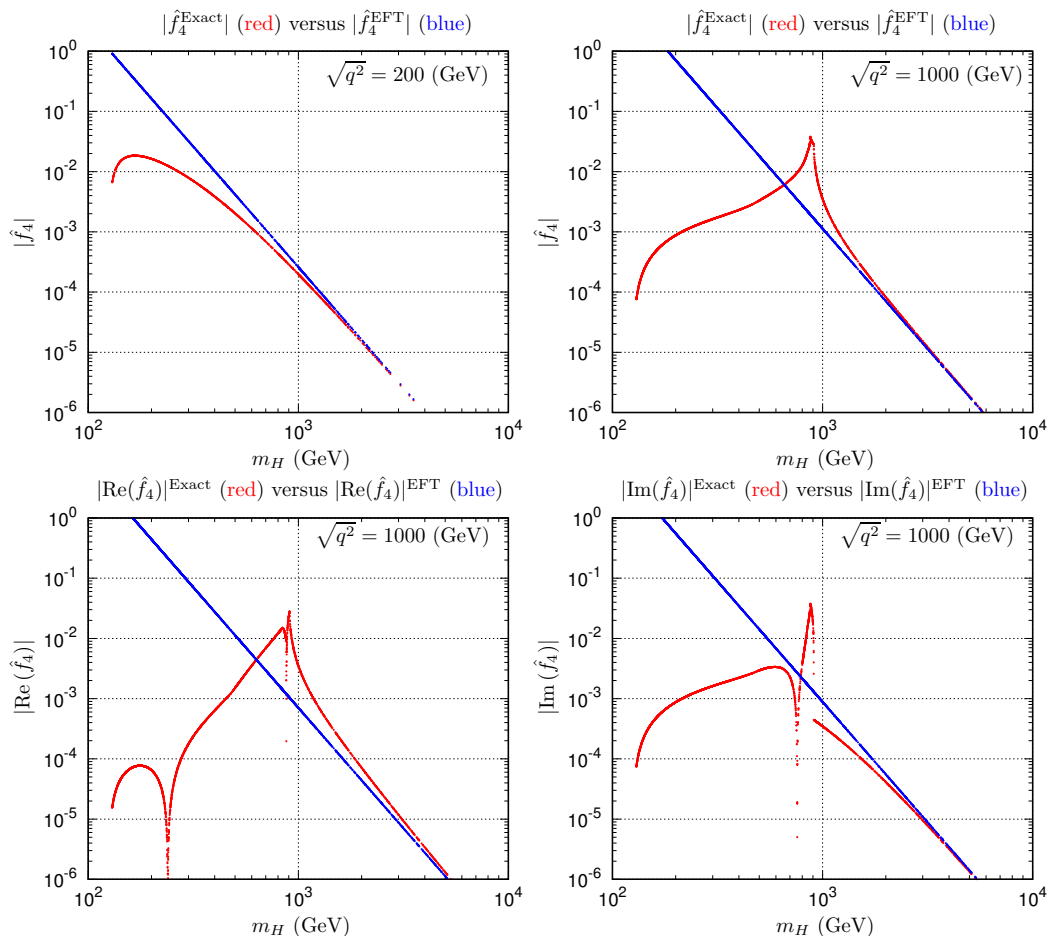


Figure 7. Red: the normalized form factor $\hat{f}_4^Z(q^2)$ as defined in eq. (4.10). We show the dependence on the second neutral Higgs mass m_H for two values of $\sqrt{q^2}$. For $\sqrt{q^2} = 1$ TeV we also show separately the real and imaginary parts (for $\sqrt{q^2} = 200$ GeV the form factor is purely real). The heaviest neutral Higgs mass is assumed to be $\sqrt{m_H^2 + v^2}$. Blue: the same observable calculated in the matched SMEFT (cf. eq. (5.1)).

We have checked numerically that eq. (5.1) correctly reproduces the f_4^Z form factor in the C2HDM in the decoupling limit. This is illustrated in figure 7 where, as long as $q^2 \ll m_H^2$, both the real and imaginary parts of the two results converge as we increase m_H .

We find that the CP violating Z^3 form factor is strongly suppressed in the decoupling limit. First, the momentum integration brings the suppression factor $1/m_H^4$ in eq. (5.1), which is stronger than the naive estimate from dimensional analysis due to cancellations between diagrams with h_2 and h_3 . Moreover, in the decoupling limit the mixing angles between the Higgs scalars are also suppressed:

$$\delta^2 x_1 x_2 x_3 \approx \frac{v^6}{2m_H^4} \text{Im}[Z_5^* Z_6^2]. \tag{5.3}$$

All in all, we find that $f_4^Z \sim \frac{1}{(16\pi^2)m_H^8}$ in the decoupling limit. This tells us that, in the SMEFT matched to C2HDM at one loop, the CP violating ZZZ vertex arises from a

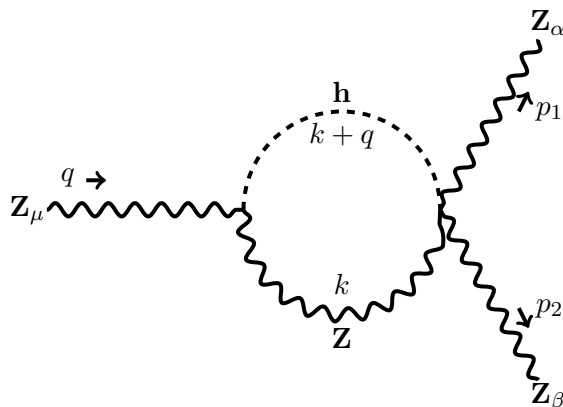


Figure 8. A one-loop diagram contributing to the Z^3 vertex in the EFT. There are two other diagrams corresponding to permutations of the external legs.

dimension-12 operator! Note that $f_4^Z(q^2)$ has an imaginary part for $q^2 > (m_Z + m_h)^2$. Indeed, the DiscB function has an imaginary part and a branch cut for $p^2 > (m_1 + m_2)^2$, while it is real for $p^2 < (m_1 + m_2)^2$. This confirms the argument above eq. (5.1) that the ZZZ vertex should arise from loop diagrams in the EFT where Z and h can simultaneously go on-shell and that the CP-violating dimension-12 operator should be present in the EFT matched at tree level to the C2HDM.

In appendix B, using the functional integral methods [30, 33], we sketch how to systematically derive the tree-level EFT Lagrangian for the C2HDM in the manifestly $SU(3) \times SU(2) \times U(1)$ gauge invariant language up to an arbitrary order in $1/m_H$ expansion. We follow that procedure and find that the leading CP-violating operator in the bosonic sector indeed occurs at $\mathcal{O}(m_H^{-8})$. The operator in question is identified as

$$\mathcal{L}_{\text{SMEFT}} \supset -\frac{Z_5^* Z_6^2}{2m_H^8} \left[D^2 \left(H^\dagger X_0 \right) H \right]^2 + \text{h.c.}, \tag{5.4}$$

where $X_0 \equiv H^\dagger H - v^2/2$. Expanding the Higgs doublet around its VEV, the operator in eq. (5.4) yields (among others) the $Z^3 h$ interaction term:

$$\mathcal{L}_{\text{SMEFT}} \supset \text{Im} \left(Z_5^* Z_6^2 \right) \left(\frac{g}{c_W} \right)^3 \frac{v^7}{8m_H^8} \partial_\nu h Z^\nu Z_\mu Z^\mu, \tag{5.5}$$

which is P-even and C-odd (thus CP-odd). Hence, the dimension-12 operator in eq. (5.4) leads to CP violation when $\text{Im} \left(Z_5^* Z_6^2 \right) \neq 0$. An equivalent way to derive the effective interaction in eq. (5.5) from the C2HDM is to consider a tree-level exchange of the heavy Higgs scalars between the ZZ and Zh vertices.

In the presence of the CP-violating interaction in eq. (5.5), one indeed finds 1-loop contributions to the Z^3 vertex, see the diagrams in figure 8. Working in the unitary gauge

we find

$$\begin{aligned}
 i\Gamma_{\mu\alpha\beta} = & i\text{Im}(Z_5^* Z_6^2) \left(\frac{g}{c_W}\right)^3 \frac{v^6}{2m_H^8} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - m_Z^2} \left\{ \right. \\
 & + \frac{m_Z^2 [\eta_{\mu\alpha}(k+q)_\beta + \eta_{\mu\beta}(k+q)_\alpha] - k_\mu [k_\alpha(k+q)_\beta + k_\beta(k+q)_\alpha]}{(k+q)^2 - m_h^2} \\
 & + \frac{m_Z^2 [\eta_{\mu\alpha}(k-p_2)_\beta + \eta_{\mu\beta}(k-p_2)_\alpha] - k_\beta [k_\alpha(k-p_2)_\mu + k_\mu(k-p_2)_\alpha + \eta_{\mu\alpha}(k^2 - kp_2)]}{(k-p_2)^2 - m_h^2} \\
 & \left. + \frac{m_Z^2 [\eta_{\mu\alpha}(k-p_1)_\beta + \eta_{\mu\beta}(k-p_1)_\alpha] - k_\alpha [k_\beta(k-p_1)_\mu + k_\mu(k-p_1)_\beta + \eta_{\mu\beta}(k^2 - kp_1)]}{(k-p_1)^2 - m_h^2} \right\} \\
 & + (\text{ILS}). \tag{5.6}
 \end{aligned}$$

Evaluating the integral in `Package-X` [47] and extracting f_4^Z , we exactly recover the result in eq. (5.1). This confirms that the dimension-12 operator in eq. (5.4) fully accounts for the leading $1/m_H$ behavior of the ZZZ vertex in the C2HDM at one loop in the decoupling limit.

It may be surprising that the Z^3 vertex in the EFT arises only at the dimension-12 level. After all, there are lower-dimensional CP-violating operators that lead to Z^3 interactions. It is well known that the Z^3 vertex cannot be generated by dimension-6 operators, however it does arise from the dimension-8 operator

$$\mathcal{L}_{D=8} \supset \frac{ic_8}{\Lambda^4} B_{\mu\nu} B^{\mu\rho} H^\dagger \{D^\nu, D_\rho\} H, \tag{5.7}$$

and other similar operators with $B_{\mu\nu} \rightarrow W_{\mu\nu}^i$ [36]. These operators lead to the contact Z^3 interaction in eq. (2.2), and thus directly contribute to the f_4^Z form factor without going through a loop diagram. However, one can prove that the dimension-8 operators like the one in eq. (5.7) cannot be generated from the C2HDM at one loop. The underlying reason is that in the C2HDM all new CP-violating effects are proportional to the Jarlskog-type invariant [27]:

$$J_{\text{CP}} \equiv \frac{(m_{h_3}^2 - m_{h_2}^2)(m_{h_3}^2 - m_{h_1}^2)(m_{h_2}^2 - m_{h_1}^2)}{m_{h_3}^2 m_{h_2}^2 m_{h_1}^2} x_1 x_2 x_3. \tag{5.8}$$

In the decoupling limit, eq. (5.3) shows that this invariant is proportional to the Higgs potential couplings Z_i in the 3rd power. The rest follows from power counting using the Planck constant \hbar as a proxy [56–60]. Reinstating the Planck constant \hbar in the path integral, $\int D\phi e^{i \int d^4x \mathcal{L}/\hbar}$, the Lagrangian should carry the dimension $[\mathcal{L}] = \hbar^1$. One can assign the power $\hbar^{1/2}$ to each propagating field, the power $\hbar^{1-n/2}$ to the coupling multiplying the term with n fields in the Lagrangian, and the power \hbar^1 for each loop factor $\frac{1}{16\pi^2}$. In this scheme, the electroweak couplings carry the power $[g] = \hbar^{-1/2}$, while for the quartic Higgs couplings $[Z_i] = \hbar^{-1}$. It follows that the CP violating invariant is proportional to $J_{\text{CP}} \sim \hbar^{-3}$. On the other hand, the Wilson coefficient of the dimension-8 operator in eq. (5.7) should have $[c_8] = \hbar^{-1}$. If that operator arises at l loops in the C2HDM then $c_8 \sim \frac{g^2 J_{\text{CP}}}{(16\pi^2)^l}$ and the \hbar power counting fixes $l = 3$: the dimension-8 operator in eq. (5.7) cannot appear before the 3 loop level in the matching of the SMEFT to the C2HDM. The same power counting shows that the dimension-12 operator in eq. (5.7) is allowed at tree level.

6 Conclusions

In this paper we have studied the CP violating triple-Z vertex in the C2HDM and in its effective description within the SMEFT framework. From the point of view of the high-energy theory, the ZZZ vertex probes one of the two independent Jarlskog-type invariants in the extended Higgs sector. The leading contributions arise from triangle one-loop diagrams with both SM particles and the new Higgs scalars. We obtained the CP violating form factor f_4^Z in a general R_ξ gauge, thus demonstrating the gauge invariance of the result and reassessing previous calculations in the literature. Starting from the (complicated) full result, we extracted an analytic approximation valid in the decoupling limit when the mass scale m_H of the heavy scalars is much larger than m_Z and the momentum flowing through the vertex. Given that approximation, we were able to identify the operators and diagrams responsible for the generation of the ZZZ vertex in the low-energy effective theory where the heavy scalars are integrated out. Even though the ZZZ vertex can in principle be generated by dimension-8 operators in the SMEFT, such contributions are absent in the effective theory matched to the C2HDM at one loop. This fact may be surprising at first, but it follows from simple power counting, given the dependence of the Jarlskog invariants on the masses and couplings of the C2HDM. Instead, we found that the CP violating ZZZ vertex appears in the effective theory only at the level of dimension-12 operators. In practice, this means the CP violating effects in diboson production will be extremely suppressed (by a loop factor multiplied by $(v/m_H)^8$) if the mass scale of the heavy Higgs partners is well above the weak scale.

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A Effective ZZZ vertex via method of regions

In this appendix we discuss how to isolate the leading contribution to the CP-violating ZZZ form factor $f_4^Z(q^2)$ in the C2HDM in the limit where the extra scalars are much heavier than the Higgs boson. To this end we will utilize the method of regions [55]. A loop integral with two disparate mass scales $m_{\text{light}} \ll m_{\text{heavy}}$ can be calculated by A) expanding the integrand for *soft* momenta $k \sim m_{\text{light}}$ and performing the integral, B) expanding the integrand for *hard* momenta $k \sim m_{\text{heavy}}$ and performing the integral, and

adding the contributions A) and B). Note that the separate soft and hard contributions may be UV or IR divergent. If that is the case, the integrals have to be regulated, with the regulator dependence canceling out when the full result is finite. In the following we will implicitly use the dimensional regularization which is convenient because the EFT expansion is not complicated by the presence of massive regulators.

We apply this method to the ZZZ vertex in the C2HDM, whose integral representation is given in eq. (4.11). For presentation purposes, in this appendix we work in the unphysical limit $m_1 = m_Z$. The reason is that in this limit the ZZZ vertex simplifies considerably, as the first four lines in eq. (4.11) cancel against each other:

$$i\Gamma_{\mu\alpha\beta} \rightarrow -im_Z^2 \left(\frac{g}{c_W}\right)^3 (x_1 x_2 x_3) \int \frac{d^4 k}{(2\pi)^4} \epsilon_{ijk} \left\{ \frac{k_\beta \eta_{\mu\alpha}}{((k-p_1)^2 - m_Z^2)((k+p_2)^2 - m_j^2)(k^2 - m_k^2)} - \frac{k_\alpha \eta_{\mu\beta}}{((k-p_1)^2 - m_j^2)((k+p_2)^2 - m_Z^2)(k^2 - m_k^2)} \right\} + (\text{ILS}) \equiv i\hat{\Gamma}_{\mu\alpha\beta}. \quad (\text{A.1})$$

Taking that simplified limit allows us to illustrate the gist of the argument. The discussion for the general case $m_1 = m_h$ is completely analogous, but much more tedious and paper-consuming.

We can rewrite eq. (A.1) as

$$i\hat{\Gamma}_{\mu\alpha\beta} = -m_Z^2(m_3^2 - m_2^2) \left(\frac{g}{c_W}\right)^3 (x_1 x_2 x_3) \left[\eta_{\mu\alpha} (I_\beta^{LH} + I_\beta^{HH}) + \eta_{\mu\beta} (\tilde{I}_\alpha^{LH} + \tilde{I}_\alpha^{HH}) \right] + (\text{ILS}). \quad (\text{A.2})$$

Here I_β^{LH} sums the contributions with one heavy scalar in the loop:

$$I_\beta^{LH} = \int \frac{d^4 k}{(2\pi)^4} \frac{ik_\beta}{((k-p_1)^2 - m_Z^2)} \times \left[\frac{1}{(k^2 - m_Z^2)((k+p_2)^2 - m_2^2)((k+p_2)^2 - m_3^2)} - \frac{1}{((k+p_2)^2 - m_Z^2)(k^2 - m_2^2)(k^2 - m_3^2)} \right], \quad (\text{A.3})$$

while I_β^{HH} sums the contributions with two heavy scalars in the loop:

$$I_\beta^{HH} = \int \frac{d^4 k}{(2\pi)^4} \frac{ik_\beta(2kp_2 + m_Z^2)}{((k-p_1)^2 - m_Z^2)(k^2 - m_2^2)(k^2 - m_3^2)((k+p_2)^2 - m_2^2)((k+p_2)^2 - m_3^2)}. \quad (\text{A.4})$$

\tilde{I}_α^{XH} is the same as I_α^{XH} with $p_2 \leftrightarrow p_1$. Note that I^{XH} have dimensions $[\text{mass}]^{-4}$.

Let us apply the method of regions to I_β^{XH} . We assume $m_2 \sim m_3 \sim m_H \gg m_Z$. Starting with I_β^{HH} , the soft limit is strongly suppressed by the heavy scalar mass, $I_\beta^{HH,\text{soft}} \sim \mathcal{O}(m_H^{-8})$. In the hard limit the suppression is less severe: $I_\beta^{HH,\text{hard}} \approx \mathcal{O}(m_H^{-4})p_{2,\beta} + \mathcal{O}(m_H^{-6})p_{1,\beta}$. Contributions to f_4^Z arise only from the second term, thus they are $\mathcal{O}(m_H^{-6})$. Turning to I_β^{LH} , its hard part scales in the same way as $I_\beta^{HH,\text{hard}}$. However, the soft part is only suppressed by m_H^{-4} :

$$I_\beta^{LH,\text{soft}} \approx \frac{i}{m_H^4} \int \frac{d^4 k}{(2\pi)^4} \frac{k_\beta}{((k-p_1)^2 - m_Z^2)} \left[\frac{1}{(k^2 - m_Z^2)} - \frac{1}{((k+p_2)^2 - m_Z^2)} \right], \quad (\text{A.5})$$

and therefore provides the leading contribution to $f_4^Z(q^2)$. The integral can be evaluated using `Package-X` [47]:

$$I_\beta^{LH,\text{soft}} \approx \frac{\sqrt{3}\pi + 3\text{DiscB}[q^2, m_Z, m_Z]}{96\pi^2 m_H^4}, \quad (\text{A.6})$$

where the function `DiscB` is defined in eq. (5.2). All in all we find

$$ef_4^Z(q^2) = -\frac{m_Z^2(m_3^2 - m_2^2)}{m_H^4} \left(\frac{g}{c_W}\right)^3 (x_1 x_2 x_3) \frac{\sqrt{3}\pi + 3\text{DiscB}[q^2, m_Z, m_Z]}{96\pi^2} + \mathcal{O}(m_H^{-6}). \quad (\text{A.7})$$

For arbitrary m_h the calculation is completely analogous. In particular, the leading contribution to f_4^Z is still $\mathcal{O}(m_H^{-4})$ and corresponds to the soft region of the diagrams with a single heavy scalar in the loop. The (much more lengthy) result in the general case is displayed in eq. (5.1). With a bit of algebra one can show that eq. (A.7) indeed corresponds to the $m_h \rightarrow m_Z$ limit of the general result.

Taking into account $x_1 x_2 x_3 \sim \mathcal{O}(m_H^{-4})$, the form factor is dramatically suppressed, $f_4^Z \sim \mathcal{O}(m_H^{-8})$. This tells us that in the low-energy EFT below the scale m_H the form factor must arise from a dimension-12 operator. Since the leading contribution to f_4^Z arises from the soft region of the integral in eq. (A.1), in the EFT it will be reproduced by a loop diagram with a single insertion of the dimension-12 operator. The same conclusion can be reached by observing that f_4^Z has a branch cut corresponding to the light scalar and Z boson in the loop simultaneously going on-shell. The responsible operator, the CP-violating vertex, and the loop diagram were identified in section 5. The hard part of eq. (A.1) corresponds to tree-level contributions of contact interactions in the EFT, but that is suppressed by an additional factor of $1/m_H^2$ and thus enters only at the level of dimension-14 operators.

B ZZZ vertex from CP-violating EFT operators

In this appendix we identify the leading CP-violating operators contributing to the ZZZ vertex in the low-energy effective theory of the C2HDM after integrating out the heavy Higgs scalars. An efficient way to proceed is to use functional methods while keeping the electroweak $SU(2) \times U(1)$ symmetry manifest. In this approach, the effective Lagrangian at tree level is given by $\mathcal{L}_{\text{EFT}}(H_1) = \mathcal{L}_{\text{C2HDM}}(H_1, H_2^c(H_1))$, where H_2^c is the solution of its classical equation of motion in the C2HDM with H_1 treated as background field. The result does not depend on which 2HDM basis is used as the starting point, however the calculation is simplest in the Higgs basis where one avoids the complications of VEV and couplings redefinitions and Zh kinetic mixing.

Solving the equation of motion and deriving \mathcal{L}_{EFT} can be readily performed perturbatively in the $1/Y_2$ expansion. As explained in section 5, power counting arguments show that the relevant CP-violating operators arise only at the level at $\mathcal{O}(Y_2^{-4})$, corresponding to dimension-12 operators. Deriving the complete effective Lagrangian up to dimension 12 would be quite a task. For the present purpose, we focus only on its small fragment containing purely bosonic CP-violating interactions. We know that these have to be proportional

to the Jarlskog-like invariant $\text{Im}(Z_5^* Z_6^2)$. Therefore we will only trace the terms in \mathcal{L}_{EFT} that contain Z_5 or Z_6 , and ignore everything else. We thus consider the C2HDM Lagrangian

$$\begin{aligned} \mathcal{L}_{\text{C2HDM}} = & |D_\mu H_1|^2 - Y_1 |H_1|^2 - \frac{Z_1}{2} |H_1|^4 \\ & + |D_\mu H_2|^2 - Y_2 |H_2|^2 - \left[(Y_3 + Z_6 |H_1|^2) H_1^\dagger H_2 + \text{h.c.} \right] - \left[\frac{Z_5}{2} (H_1^\dagger H_2)^2 + \text{h.c.} \right] + \dots, \end{aligned} \quad (\text{B.1})$$

where the dots stand for other terms in the Higgs potential, gauge kinetic terms, and all fermionic terms, which are not relevant for the present discussion. We work in the Higgs basis where $Y_3 = -Z_6 v^2/2$, $\langle H_1 \rangle = v/\sqrt{2}$, $\langle H_2 \rangle = 0$. Then $Y_3 + Z_6 |H_1|^2 = Z_6 X_0$, where we defined $X_0 \equiv |H_1|^2 - v^2/2$. The equation of motion for H_2 takes the form

$$Y_2 H_2 + D^2 H_2 + Z_6^* X_0 H_1 + Z_5^* (H_2^\dagger H_1) H_1 + \dots = 0. \quad (\text{B.2})$$

We search for a perturbative solution in the form $H_2^c = \sum_{n=1}^{\infty} Y_2^{-n} H_2^{(n)}$. This leads to the recursive system of equations:

$$\begin{aligned} H_2^{(1)} &= -Z_6^* X_0 H_1 + \dots, \\ H_2^{(n+1)} &= -D^2 H_2^{(n)} - Z_5^* (H_2^{(n)\dagger} H_1) H_1 + \dots, \end{aligned} \quad (\text{B.3})$$

which determines H_2^c (or at least its part depending on Z_5 and Z_6) to an arbitrary order n . We will only need the explicit solution up to $n = 4$:

$$\begin{aligned} H_2^{(2)} &= Z_6^* D^2 (X_0 H_1) + Z_5^* Z_6 X_0 |H_1|^2 H_1 + \dots, \\ H_2^{(4)} &= D^4 H_2^{(2)} + Z_5^* D^2 [(H_2^{(2)\dagger} H_1) H_1] + Z_5^* (D^2 H_2^{(2)\dagger} H_1) H_1 + |Z_5|^2 |H_1|^2 (H_1^\dagger H_2^{(2)}) H_1 + \dots \end{aligned} \quad (\text{B.4})$$

Plugging that solution back into eq. (B.1) one gets the EFT Lagrangian in $1/Y_2$ expansion: $\mathcal{L}_{\text{EFT}} = \mathcal{L}_{\text{SM}} + \sum_{n=1}^{\infty} Y_2^{-n} \mathcal{L}^{(2n+4)}$, where each term contains local operators composed of H_1 and its (covariant) derivatives. In the low-energy theory H_2 is integrated out and H_1 remains as the only doublet scalar, so in the following we relabel $H_1 \rightarrow H$. It is now a trivial if tedious exercise to determine the EFT operators $\mathcal{L}^{(2n+4)}$ at each given order. For example, this procedure yields $\mathcal{L}^{(6)} \supset |Z_6|^2 X_0^2 |H|^2$ which shifts the triple Higgs boson coupling away from the SM prediction, or $\mathcal{L}^{(8)} \supset |Z_6 D_\mu (X_0 H)|^2$ which renormalizes the Higgs boson kinetic terms, thus uniformly shifting all the Higgs boson couplings. At $n = 8$ we also encounter a term proportional to $Z_5^* Z_6^2$, $\mathcal{L}^{(8)} \supset -\frac{Z_5^* Z_6^2 X_0^2 |H|^4}{2} + \text{h.c.}$, but it is CP-conserving and only yields interactions proportional to $\text{Re} Z_5^* Z_6^2$. At $n = 10$ we find $\mathcal{L}^{(10)} \supset -\frac{Z_5^* Z_6^2 D_\mu (H^\dagger X_0) D_\mu (X_0 |H|^2 H)}{2} + \text{h.c.}$, but the only resulting interactions proportional to $\text{Im} Z_5^* Z_6^2$ are of the form $\sim h^m \partial_\mu Z^\mu$ with $m \geq 3$, which is not interesting for our purpose. The first time we encounter a genuine CP-violating interaction proportional to $\text{Im} Z_5^* Z_6^2$ is in $\mathcal{L}^{(12)}$. At that order the effective Lagrangian can be written as

$$\begin{aligned} \mathcal{L}^{(12)} = & -\frac{1}{2} H_2^{(2)\dagger} D^2 H_2^{(2)} - H_2^{(1)\dagger} D^2 H_2^{(3)} - H_2^{(1)\dagger} H_2^{(4)} - H_2^{(2)\dagger} H_2^{(3)} \\ & - Z_6 X_0 H^\dagger H_2^{(4)} - \frac{Z_5}{2} (H^\dagger H_2^{(2)})^2 - Z_5 (H^\dagger H_2^{(1)}) (H^\dagger H_2^{(3)}) + \text{h.c.} \\ = & \frac{1}{2} H_2^{(2)\dagger} D^2 H_2^{(2)} - Z_6 X_0 H^\dagger H_2^{(4)} + \frac{Z_5}{2} (H^\dagger H_2^{(2)})^2 + \text{h.c.} + \dots \end{aligned} \quad (\text{B.5})$$

To derive the second equality we used the recursion in eq. (B.3). Plugging in the solution in eq. (B.4) and integrating by parts we find that $\mathcal{L}^{(12)}$ contains the following terms proportional to $Z_5^* Z_6^2$:

$$\mathcal{L}^{(12)} \supset -Z_5^* Z_6^2 \left[D^2(H^\dagger X_0) D^2(X_0 |H|^2 H) + \frac{1}{2} \left(D^2(H^\dagger X_0) H \right)^2 \right] + \text{h.c.} \quad (\text{B.6})$$

Ignoring again interactions proportional to $\partial_\mu Z^\mu$, only the second term in the bracket leads to non-trivial CP-violating interactions:

$$\begin{aligned} \mathcal{L}^{(12)} &\supset \text{Im} \left(Z_5^* Z_6^2 \right) \frac{g v^6}{2c_W} Z^\nu \partial_\nu h \square h + \mathcal{O}(Z h^3) \\ &\rightarrow \text{Im} \left(Z_5^* Z_6^2 \right) \frac{g v^5}{2c_W} \partial_\nu h Z^\nu \left(m_Z^2 Z_\mu Z^\mu + 2m_W^2 W_\mu^+ W^{\mu-} \right). \end{aligned} \quad (\text{B.7})$$

In the last step we used the classical equation of motion for the Higgs boson field. These are the leading CP-violating interactions in the bosonic sector of the low-energy effective theory of C2HDM. At one loop in the EFT, the interaction term $\sim \partial_\nu h Z^\nu Z_\mu Z_\mu$ generates the CP-violating ZZZ vertex via the Feynman diagram in figure 8.

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