Gauge and Yukawa coupling beta functions of two-Higgs-doublet models to three-loop order

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Abstract

We compute the beta functions for the three gauge couplings and the Yukawa matrices of a general two-Higgs-doublet model in the modified minimal subtraction scheme to three loops. The calculations are performed using Lorenz gauge in the unbroken phase. We discuss in detail the occurence of poles in anomalous dimensions and propose practical prescriptions to avoid them. We provide explicit results for the often used $\mathbb{Z}_2$-symmetric versions of the two-Higgs-doublet model of type I, II, X and Y. Furthermore, we provide the first independent cross-check of the three-loop Yukawa coupling beta functions of the Standard Model.

1 Introduction

An appealing renormalization scheme for the couplings of the Standard Model of particle physics (SM) and of its extensions is the minimal modified subtraction ($\overline{\text{MS}}$) scheme. As a consequence, the numerical values of the couplings depend on the renormalization scale μ, which in general is of the same order as the energy scale of the considered process. The values of the couplings at different scales are related by so-called beta functions which in perturbation theory are given as power series in all couplings of the theory.

In the SM there are three gauge couplings (g_1, g_2, g_s), the quartic Higgs boson coupling λ, and a Yukawa coupling for each massive fermion, where often only the third generation couplings, y_t, y_b, and y_τ are considered as non-zero. For all couplings the three-loop beta functions have been completed recently: the gauge coupling beta functions have been computed in Refs. [1–3], the ones for the Yukawa couplings in Refs. [4–6] and λ has been considered in [7,8]. Leading terms to the four-loop QCD beta function and the Higgs self coupling involving the top Yukawa coupling and α_s have been computed in Refs. [9–12] and within QCD the beta function is even known to five loops [13–15].

There are a number of two-loop results which can be immediately adapted to a large class of non-supersymmetric beyond-the-SM theories. In particular, two-loop results for gauge [16], Yukawa [17] and scalar self couplings [18] are known since middle of the eighties. Furthermore, the three-loop gauge coupling beta function for a simple gauge group has been calculated [19]. In this work we consider the so-called two-Higgs-doublet model (2HDM) and compute the gauge and Yukawa coupling beta functions to three-loop order.

2HDMs, where the SM Higgs sector is extended by a second $SU(2)$ Higgs doublet, are attractive extensions of the SM. Although simple and probably not realized in nature in its minimal version, 2HDMs nevertheless constitute prototype-extensions of the SM which can be used to study several features of beyond-SM theories. In particular, for a certain choice of parameters it implements the Higgs sector of the Minimal Supersymmetric Standard Model. Further motivation and several phenomenological applications can be found in the review [20].

The most general 2HDM has many parameters and furthermore several unwanted features like flavour-changing neutral currents (FCNCs) at tree level. Thus, often additional symmetries are imposed. For example, if CP conservation in the Higgs sector is assumed one has five physical scalar degrees of freedom which correspond to two scalar, one pseudo scalar and a charged Higgs boson. In these models, both Higgs doublets acquire vacuum expectation values v_1 and v_2 such that $v = \sqrt{v_1^2 + v_2^2} \simeq 246$ GeV determines the $W^\pm$ and Z boson masses in the same way as in the SM. The ratio v_2/v_1 is denoted by $\tan\beta$.

The scope of the present work is twofold: First, we provide the first independent cross check of the three-loop Yukawa coupling beta functions in the SM. In this context it is particularly important to carefully investigate the scheme used for γ_5 in $D \neq 4$ dimensions. Note that for the gauge couplings it is possible to choose Green's functions without ex-

ternal fermions. For Yukawa couplings this is not possible anymore. As a second aim, we extend both the gauge and Yukawa beta functions to a general 2HDM. There is no change in the underlying integrals, which have to be evaluated, however, there are conceptional challenges in connection to the wave function renormalization of the scalar fields.

The remainder of the paper is organized as follows: In the next section we introduce the 2HDM which serves to fix the notation. Section 3 is devoted to technical details. In particular, we introduce the renormalization constants for the parameters and fields and define the beta functions and anomalous dimensions which we want to compute. The main focus of Section 4 relies on the proper definition of the renormalization constants such that the anomalous dimensions are finite. We investigate this problem in detail and propose practical solutions. A detailed discussion of the computation of the gauge and Yukawa coupling beta functions is provided in Sections 5 and 6, respectively. In these Sections we also explain how one can arrive at special versions of the 2HDM and the SM results. Furthermore, we compare the Yukawa beta functions to Ref. [4]. The findings of this paper are summarized in Section 7.

2 Two-Higgs-doublet model

An extensive discussion of a general 2HDM model can be found in Ref. [20]. For convenience we repeat in the following the features which are important for our calculation.

The additional Higgs doublet leads to an enlarged Yukawa sector which can be written as

$$\mathcal{L}_Y = - \left(\sum_{i=a}^{2} \bar{Q}_L \tilde{\Phi}_a Y_a^u u_R + \bar{Q}_L \Phi_a Y_a^d d_R + \bar{L}_L \Phi_a Y_a^l l_R + \text{h.c.} \right) . \tag{1}$$

The sum runs over the two doublets and "h.c." refers to the hermitian conjugate part. Y_a^u, Y_a^d and Y_a^l are generic 3×3 complex matrices containing the Yukawa couplings and Q_L, L_L, u_R, d_R and l_R represent left- and right-handed quark and lepton fields. $\tilde{\Phi} = i\tau_2 \Phi_j^*$ is the charge conjugated doublet with τ_2 being the second Pauli matrix.

The 2HDM has furthermore a more involved scalar potential which in its general form is given by [21]

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

The parameters m_{11}^2, m_{22}^2 and λ_1, ..., λ_4 are real whereas in general m_{12}^2, λ_5, λ_6 and λ_7 are complex. This leads to fourteen degrees of freedom, eleven of which are physical as can be seen by an appropriate basis choice for Φ_1 and Φ_2 [20].

As in all multi-Higgs-doublet models, the Lagrange densities given in Eqs. (1) and (2) contain FCNCs. For example, the up-type Yukawa matrices Y_1^u and Y_2^u will not be in general simultaneously diagonalizable and thus neutral Higgs scalars ϕ will mediate FCNCs of the form $\bar{u}u'\phi$ already at the tree level, where $u \neq u'$ are two different up-type quarks. To avoid FCNCs at tree level [22, 23] it is necessary that all fermions with the same quantum numbers couple to one and the same Higgs multiplet. This condition can be satisfied if all quarks couple to just one of the Higgs doublets or the right-handed up- and down-type quarks couple to different Higgs doublets. Depending on whether the right-handed leptons couple to the Higgs doublets in the same manner as the right-handed down-type quarks, or in the opposite way, further two possibilities can be identified. The resulting four models are summarized in Tab. 1. They can be realized by imposing a $\mathbb{Z}_2$ symmetry to the general model. In fact, the type I 2HDM can be obtained by enforcing an additional $\mathbb{Z}_2$ symmetry under which the theory has to be invariant namely $\Phi_1 \to -\Phi_1$ and $\Phi_2 \to \Phi_2$. The type II 2HDM can be derived via the symmetries $\Phi_1 \to -\Phi_1$, $\Phi_2 \to \Phi_2$, $d_R \to -d_R$ and $l_R \to -l_R$. The additional discrete symmetries required for the other two models can be derived similarly. Note that the $\mathbb{Z}_2$ symmetries require that $m_{12} = \lambda_6 = \lambda_7 = 0$.

In a generic quark basis as given in Eq. (1) the condition for non-existence of FCNCs in the up-type (down-type) quark sector is that the Yukawa matrices Y_1^u and Y_2^u (Y_1^d and Y_2^d) commute [24]. If one of the two Yukawa matrices is zero, as it is actually the case for the four models shown in Tab. 1, this condition is trivially fulfilled.

The most general Lagrange densities in Eqs. (1) and (2) contain several fields with the same quantum numbers that can mix. Therefore, one can rewrite the Lagrangian in terms of the new fields obtained from the original ones by simple basis transformations. In the following we will refer to these transformations as flavour transformations for both fermions and scalars. Obviously, the physical observables do not depend on such redefinitions. They can depend only on quantities that are invariant under arbitrary unitary flavour transformations. Ideally, one would be able to express the fundamental Lagrangian parameters in terms of these invariants. However, some of the Lagrangian parameters in Eq. (1), that do not take into account flavour symmetries are not physical. That is, there are Lagrangian parameters that can be expressed as linear combinations of others. This also means that there is a basis where the unphysical parameters are identically zero, i.e. one can rotate them away via flavour transformations. In other words, any coupling or mixing angle can be expressed in terms of so-called flavour invariants. This statement has been explicitly proven for the Yukawa sector of the SM [25] and for the scalar sector of the 2HDM, for example, in Refs. [26, 27].[1] In this paper, we (re)confirm the findings of [25–27] explicitly for the Yukawa sector of the SM and for $\mathbb{Z}_2$-symmetric 2HDMs through three loops.

The flavour transformations for fermion and scalar fields of the in Lagrangian Eq. (1) can

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[1]For more details see Ref. [20] and references therein.

Type	u_R	d_R	l_R
I	Φ_2	Φ_2	Φ_2
II	Φ_2	Φ_1	Φ_1
X	Φ_2	Φ_2	Φ_1
Y	Φ_2	Φ_1	Φ_2

Table 1: Four $\mathbb{Z}_2$-symmetric 2HDMs. The table shows which right-handed fermion field couples to which doublet.

be summarized as follows

$$
\begin{aligned}
Q'_{L,I} &= U_{Q,IK} Q_{L,K} \,, \\
u'_{R,i} &= U_{u,ik} u_{R,k} \,, \\
d'_{R,m} &= U_{d,mp} d_{R,p} \,, \\
\Phi'_a &= U_{\Phi,ac} \Phi_c \,,
\end{aligned}
\tag{3}
$$

where U_Q, U_u and U_d are unitary 3×3 matrices and U_Φ is a unitary 2×2 matrix. Under these unitary basis transformations, the gauge and kinetic terms are unchanged and $\mathcal{L}_Y$ in Eq. (1) is invariant if the Yukawa matrices transform as

$$
\begin{aligned}
Y^{d\prime}_{a,Im} &= U_{Q,IK} Y^d_{b,Kp} U^\dagger_{d,pm} U^\dagger_{\Phi,ba} \\
Y^{u\prime}_{a,Ij} &= U_{Q,IK} Y^u_{b,Kl} U^\dagger_{u,lj} U^{\mathrm{T}}_{\Phi,ba}.
\end{aligned}
\tag{4}
$$

In a similar manner, one can derive the transformation properties of the parameters in the potential under redefinitions of the scalar fields [20]. One introduces the rank two and four tensors, K_{ab} and $\lambda_{ab,cd}$, so that

$$
V(\Phi_1,\Phi_2) = K_{ab}\Phi_a^\dagger\Phi_b + \frac{1}{2}\lambda_{ab,cd}(\Phi_a^\dagger\Phi_b)(\Phi_c^\dagger\Phi_d)\,,
\tag{5}
$$

with

$$
K_{ab} = K^*_{ba}\,, \quad \lambda_{ab,cd} = \lambda_{cd,ab}\,, \quad \lambda_{ab,cd} = \lambda^*_{ba,dc}\,.
\tag{6}
$$

One can match with the standard notation given in Eq. (2) and obtain the following relations

$$
\begin{aligned}
K_{11} &= m_{11}^2\,, & K_{12} &= -m_{12}^2\,, & K_{21} &= -(m_{12}^2)^*\,, \\
\lambda_{11,11} &= \lambda_1\,, & \lambda_{22,22} &= \lambda_2\,, & \lambda_{11,22} &= \lambda_{22,11} = \lambda_3\,, \\
\lambda_{12,21} &= \lambda_4\,, & \lambda_{12,12} &= \lambda_5\,, \\
\lambda_{11,12} &= \lambda_6\,, & \lambda_{22,12} &= \lambda_7\,.
\end{aligned}
\tag{7}
$$

The two tensors transform under the basis change given in Eq. (3) as

$$
K'_{ab} = U_{\Phi,a\alpha} K_{\alpha\beta} U^\dagger_{\Phi,\beta b}\,,
$$

$$\lambda'_{ab,cd} = U_{\Phi,a\alpha}U_{\Phi,c\rho}\lambda_{\alpha\beta,\rho\sigma}U^\dagger_{\Phi,\beta b}U^\dagger_{\Phi,\sigma d}. \tag{8}$$

Since the calculation of the $\overline{\text{MS}}$ renormalization constants can be performed in the unbroken phase the dimensionful parameters m_{ij} are irrelevant and thus for our calculation of the beta functions only the second transformation in Eq. (7) will be of interest.

Within the SM the physical Yukawa couplings are defined via the diagonalization of the hermitian matrices

$$M_{u,1} = Y_1^u Y_1^{u\dagger} = U_{uL,1}D_{u,1}^2 U^\dagger_{uL,1}, \quad Y_1^{u\dagger}Y_1^u = W_{uR,1}D_{u,1}^2 W^\dagger_{uR,1}, \tag{9}$$

where $U_{uL,1}$ and $W_{uR,1}$ are unitary matrices that act on the left- and right-handed up-type quark fields as introduced in Eq. (3)

$$Q_L \to U_{uL,1}Q_L, \quad u_R \to W_{uR,1}u_R, \tag{10}$$

and $D_{u,1}$ is a diagonal matrix with positive eigenvalues. Then

$$Y_1^u = U_{uL,1}D_{u,1}W^\dagger_{uR,1}, \quad \text{with} \quad D_{u,1} = \text{diag}(y_{u,1}, y_{c,1}, y_{t,1}), \tag{11}$$

where the diagonal elements of $D_{u,1}$ are the physical couplings and correspond to the positive square roots of the eigenvalues of $Y_1^u Y_1^{u\dagger}$. We can define the unitary matrices U_{dL} and W_{dR} in a similar way and decompose Y_1^d as

$$Y_1^d = U_{dL,1}D_{d,1}W^\dagger_{dR,1}, \quad \text{with} \quad D_{d,1} = \text{diag}(y_{d,1}, y_{s,1}, y_{b,1}), \tag{12}$$

i.e., Y_1^d is diagonalized via

$$Q_L \to U_{dL,1}Q_L, \quad d_R \to W_{dR,1}d_R. \tag{13}$$

However, Eqs. (10) and (13) are in conflict with each other and only one of the Yukawa matrices can be diagonalized. This leads to the definition of the CKM matrix, which, in the basis where the up-type Yukawa matrix is diagonal, is given by $V = U^\dagger_{uL,1}U_{dL,1}$. Note that $(2n-1) \overset{n=3}{=} 5$ unphysical phases can be eliminated from V via further quark field redefinitions.

The discussion up to now is in analogy to the SM. Within a general 2HDM the unitary transformations discussed above do not necessarily simultaneously diagonalize the other two Yukawa matrices Y_2^u and Y_2^d. We can still define the additional set of (non physical) Yukawa couplings as the positive square roots of the eigenvalues of the matrices

$$\begin{aligned} M_{u,2} &= Y_2^u Y_2^{u\dagger} = U_{uL,2}D_{u,2}^2 U^\dagger_{uL,2} & \text{with} \quad D_{u,2} = \text{diag}(y_{u,2}, y_{c,2}, y_{t,2}), \\ M_{d,2} &= Y_2^d Y_2^{d\dagger} = U_{dL,2}D_{d,2}^2 U^\dagger_{dL,2} & \text{with} \quad D_{d,2} = \text{diag}(y_{d,2}, y_{s,2}, y_{b,2}). \end{aligned} \tag{14}$$

To summarize, using the unitary rotations in Eq. (10) the set of Yukawa matrices transform as

$$Y_1^u \to D_{u,1}, \qquad\qquad Y_1^d \to V^\dagger D_{d,1},$$

$$Y_2^u \to N_u = U_{uL,1}^\dagger Y_2^u W_{uR,1}, \quad Y_2^d \to N_d = V^\dagger U_{dL,1}^\dagger Y_2^u W_{dR,1}, \tag{15}$$

where N_u and N_d are complex $3{\times}3$ matrices. Note that for the special case of a 2HDM with a $\mathbb{Z}_2$-symmetry only two of the four matrices in Eq. (15) are non-zero. Their eigenvalues define the physical parameters and their mixing matrix is defined in analogy to the CKM matrix in the SM.

We want to stress that within the SM and the four $\mathbb{Z}_2$-symmetric 2HDMs (cf. Tab. 1) the physical Yukawa couplings are defined as eigenvalues of the Yukawa matrices and thus, by construction, are invariant under quark flavour transformations. However, in a general 2HDM only appropriate linear combinations of the eigenvalues of the Yukawa matrices become invariant under unitary transformations of the scalar fields and can be interpreted as physical Yukawa couplings.

The strategy to construct flavour invariants in the Yukawa sector consists in taking products of Yukawa matrices, contracting over the internal flavour indices, and taking the trace over the external flavour indices. For example, the simplest flavour invariants that can be constructed within a 2HDM read

$$I_u^{(1)} = \mathrm{Tr}(Y_1^u Y_1^{u\dagger} + Y_2^u Y_2^{u\dagger}), \quad I_d^{(1)} = \mathrm{Tr}(Y_1^d Y_1^{d\dagger} + Y_2^d Y_2^{d\dagger}), \tag{16}$$

where Tr denotes the trace over the open indices of the left-handed fermions Q_L. In a generic 2HDM the matrices

$$M_u = Y_1^u Y_1^{u\dagger} + Y_2^u Y_2^{u\dagger} \quad \text{and} \quad M_d = Y_1^d Y_1^{d\dagger} + Y_2^d Y_2^{d\dagger} \tag{17}$$

are invariant under scalar flavour transformations and one can thus construct other nine flavour invariants similar to those for the SM [25, 28]. Using Section 3.1 of [25] and adapting the notation (i.e. replacing U and D by M_u and M_d) leads to

$$\begin{aligned}
I_1 &= \mathrm{Tr}(M_u), & I_3 &= \mathrm{Tr}(\tilde{M}_u), & I_6 &= \det(M_u), \\
I_2 &= \mathrm{Tr}(M_d), & I_4 &= \mathrm{Tr}(\tilde{M}_d), & I_8 &= \det(M_d), \\
I_5 &= \mathrm{Tr}(M_u M_d), & I_7 &= \mathrm{Tr}(M_d \tilde{M}_u), & I_9 &= \mathrm{Tr}(M_u \tilde{M}_d), \\
I_{10} &= \mathrm{Tr}(\tilde{M}_u \tilde{M}_d), & I_{11} &= -\frac{3i}{8}\det([M_u, M_d]),
\end{aligned} \tag{18}$$

where $\tilde{M} = M^{-1}\det(M)$. All $\mathbb{Z}_2$-symmetric 2HDMs have the same eleven invariants as the SM.

In a generic 2HDM further higher rank invariants can be constructed using tensorial properties of the Yukawa matrices. For example, the simplest additional type of rank four invariant tensors are

$$T_{uu}^{(2)} = \sum_{a,b}^{1,2} \mathrm{Tr}(Y_a^u Y_b^{u\dagger})\mathrm{Tr}(Y_b^u Y_a^{u\dagger}), \tag{19}$$

and

$$T_{dd}^{(2)} = \sum_{a,b}^{1,2} \text{Tr}(Y_a^d Y_b^{d\dagger})\text{Tr}(Y_b^d Y_a^{d\dagger}) \,, \tag{20}$$

and similar ones where Tr is replaced by the determinant. A systematic analysis of all independent invariants for a general 2HDM is, however, beyond the scope of this article.

Let us also mention at this point that the definitions for the physical Yukawa couplings and mixing matrices introduced above holds to all orders in perturbation theory.

3 Technicalities

In this work we compute the beta functions of the three gauge couplings and the Yukawa matrices in the $\overline{\text{MS}}$ scheme.

Our calculation of the beta functions are based on the Lagrange densities in Eqs. (1) and (2). The specification to the types I, II, X, and Y is straightforward. Note that the $\overline{\text{MS}}$ renormalization constants can be computed in the unbroken phase since they do not depend on the particle masses.

It is convenient to denote the gauge couplings by α_1, α_2 and $\alpha_3 = \alpha_s$, where $\alpha_i = g_i^2/(4\pi)$ and Y_a^f with $f = u, d, l$ and $a = 1, 2$ (labeling the scalar doublets). Furthermore, we introduce $\hat{\lambda}_{ab,cd} = \lambda_{ab,cd}/(4\pi)$ $(a, b, c, d = 1, 2)$, where $\lambda_{ab,cd}$ are the quartic coupling in the scalar potential. We define the beta functions via

$$\mu^2 \frac{d}{d\mu^2} \frac{\alpha_i}{\pi} = \beta_i(\{\alpha_j, Y_a^f, \lambda_{ab,cd}\}, \epsilon) \,,$$

$$\mu \frac{d}{d\mu} Y_a^f = \beta_{f,a}(\{\alpha_j, Y_a^f, \lambda_{ab,cd}\}, \epsilon) \,,$$

$$\mu^2 \frac{d}{d\mu^2} \frac{\hat{\lambda}_{ab,cd}}{\pi} = \beta_{ab,cd}(\{\alpha_j, Y_a^f, \lambda_{ab,cd}\}, \epsilon) \,, \tag{21}$$

where $\epsilon = (4 - d)/2$. Note that the dependence of the couplings on the renormalization scale is suppressed. The equations defining the beta function for Yukawa matrices have to be understood as matrix equations in flavour space. The gauge couplings are related to the fine structure constant, the weak mixing angle and the strong coupling as follows

$$\alpha_1 = \frac{5}{3} \frac{\alpha_{\text{QED}}}{\cos^2 \theta_W} \,,$$

$$\alpha_2 = \frac{\alpha_{\text{QED}}}{\sin^2 \theta_W} \,, \tag{22}$$

$$\alpha_3 = \alpha_s \,,$$

8

where the SU(5) normalization has been adopted which leads to the factor 5/3 in the definition of α_1. For models where the first and second generation Yukawa couplings are neglected, it is convenient to introduce $\alpha_{f,i} = y_{f,i}^2/(4\pi)$ with $f = b, t, \tau$ and $i = 1, 2$.

The beta functions are obtained from the renormalization constants relating bare and renormalized couplings. For the gauge couplings we have

$$\alpha_i^{\text{bare}} = \mu^{2\epsilon} Z_{\alpha_i}(\{\alpha_j\}, \epsilon)\alpha_i \,. \tag{23}$$

From this equation one obtains the following explicit formula for the beta functions after taking into account that the α_i^{bare} do not depend on μ

$$\beta_i = -\left[\epsilon\frac{\alpha_i}{\pi} + \frac{\alpha_i}{Z_{\alpha_i}} \sum_{j=1, j\neq i} \frac{\partial Z_{\alpha_i}}{\partial \alpha_j}\beta_j\right] \left(1 + \frac{\alpha_i}{Z_{\alpha_i}}\frac{\partial Z_{\alpha_i}}{\partial \alpha_i}\right)^{-1} \,. \tag{24}$$

The first term in the first factor of Eq. (24) originates from the term $\mu^{2\epsilon}$ in Eq. (23) and vanishes in four space-time dimensions. Equations (23) and (24) hold for the Yukawa couplings only for models where the Yukawa matrices are diagonal, e.g., in case only the third generation Yukawa couplings are taken into account.

The generalization of Eq. (24) to incorporate tensor-like couplings, like the Yukawa matrices and quartic couplings, is straightforward to derive. However, care has to be taken when computing derivatives of renormalization constants. Furthermore, the relations between Yukawa matrix and quartic coupling beta functions and the corresponding renormalization constants take a slightly different form than in Eq. (24), since in general, due to the tensorial nature, it is not possible to compute the inverse of the renormalization constants. For more details see Ref. [29].

Another option would be to derive the scale dependence of the eigenvalues of the Yukawa matrices and quartic couplings starting from the definition in Eq. (21).

Note that the one-loop results of Z_{α_i} only contain α_i, whereas at two loops all other couplings are present except for the quartic couplings. The renormalization constants of the Yukawa matrices contain all couplings except the quartic couplings already at one-loop order, while the quartic couplings enter at two loops. Therefore, it is necessary to compute the renormalization constants and beta functions of the quartic couplings only at one-loop order.[2]

For our calculation we use the automated setup developed for the calculation of the SM gauge beta functions to three loops [1,2]. For convenience we repeat the flowchart which illustrates the interaction of the various program packages in Fig. 1.

In a first step we implement the unbroken version of the general 2HDM discussed in Section 2 in the package `FeynRules` [31] which generates a model file for `FeynArts` [32]. The program `FeynArtsToQ2E` [33] works on the model file and translates it into input files for `QGRAF` [34] and `q2e` [35–37]. `QGRAF` is used for the generation of the amplitudes

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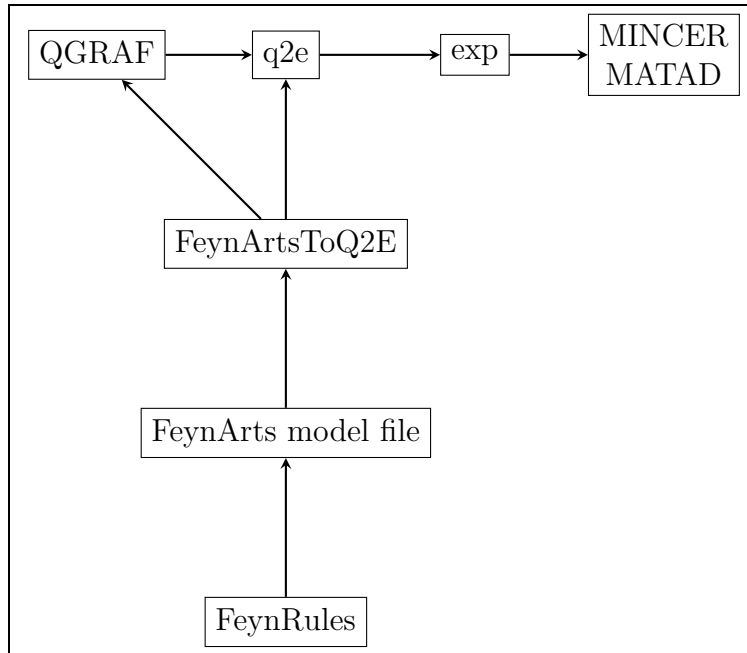[2]Our results can be found in the ancillary files to this paper [30].

Figure 1: Flowchart illustrating the workflow used for the calculation of the two- and three-point functions.

which are translated by `q2e` and `exp` [35–37] to `FORM` [38] code. The latter is processed by `MINCER` [39] and/or `MATAD` [40] which compute the Feynman integrals and outputs the ϵ expansion of the result.

For the first part of the calculation up to the generation of the input files for `QGRAF` and `q2e` no parallelization is necessary. The individual steps take at most a few minutes. However, the parallelization of the horizontal part of the flowchart (cf. Fig. 1) is essential since for some of the Green's function we have to deal with several hundred thousands of diagrams. Once `QGRAF` has produced the output file all following steps can be applied in parallel to blocks of diagrams which typically contain 1000 Feynman amplitudes.

We perform the calculation in Lorenz gauge using general gauge parameters for each gauge group. It is an important cross check that they drop out in the expressions for the renormalization constants (and beta functions) of the gauge and Yukawa couplings.

The described setup is used to compute various $\overline{\text{MS}}$ renormalization constants for fields and vertices. They are required for the construction of the renormalization constants for the gauge, Yukawa and quartic couplings.

For the SM and 2HDM with $\mathbb{Z}_2$-symmetry, one can perform the calculation in a basis where all the Yukawa matrices are diagonal and the elements of the CKM matrix are present only in the vertices containing charged currents. In such a basis, the Lagrangian parameters are physical parameters and the number of free parameters is reduced to the

2-point functions				3-point functions			
# loops	1	2	3	# loops	1	2	3
BB	16	450	49 256	BBB	44	2 472	401 460
$W_3 W_3$	19	534	57 665	$c_g \bar{c}_g g$	2	66	3 722
gg	9	170	13 671	$c_{W_1} \bar{c}_{W_2} W_3$	2	117	11 849
$c_g \bar{c}_g$	1	12	447	$\Phi_1^0 \Phi_1^{0*} W_3$	22	2 538	417 759
$c_{W_3} \bar{c}_{W_3}$	2	46	2 880	$\Phi_1^0 \Phi_2^{0*} W_3$	12	1 274	—
$q \bar{q}$	11	659	75 980	$\Phi_2^0 \Phi_1^{0*} W_3$	12	1 274	—
$l \bar{l}$	10	567	63 853	$\Phi_2^0 \Phi_2^{0*} W_3$	22	2 538	—
$\Phi_1^{0*} \Phi_1^0$	8	436	47 613	$d \bar{d} \Phi_i^0$	17	2 622	493 742
$\Phi_1^{0*} \Phi_2^0$	4	224	28 648	$u \bar{u} \Phi_i^{0*}$	17	2 622	493 742
$\Phi_2^{0*} \Phi_1^0$	4	224	28 648	$l \bar{l} \Phi_i^0$	16	2 337	426 741
$\Phi_2^{0*} \Phi_2^0$	8	436	47 613				

Table 2: The number of Feynman diagrams contributing to the one-, two- and three-loop Green's functions evaluated in this work. We computed the Yukawa vertices for both Φ_1 and Φ_2. Note that for some Green's functions less diagrams had to be calculated than in [2] since we only considered one fermion generation with matrix-like Yukawa couplings. We did not compute three-loop corrections to the vertices $\Phi_i^0 \Phi_j^{0*} W_3$ with $ij = 12, 21$ and 22. The corresponding two-loop results are needed for the three-loop calculation of $\Phi_1^0 \Phi_1^{0*} W_3$.
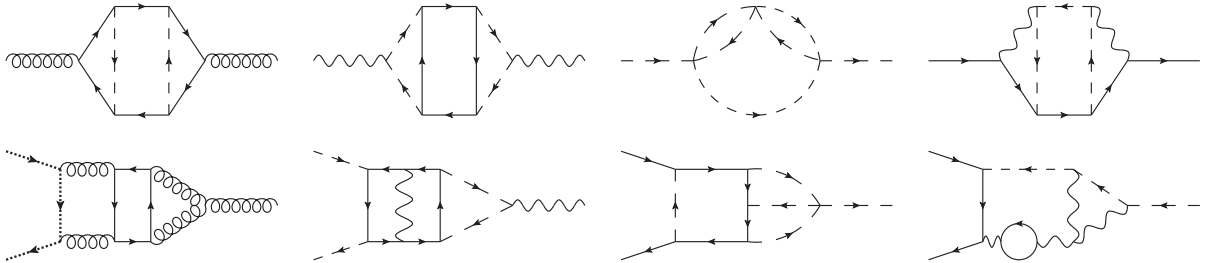

Figure 2: Sample Feynman diagrams contributing to the Green's functions which have been used for our calculation of the gauge and Yukawa coupling renormalization constants. Solid, dashed, dotted, curly and wavy lines denote fermions, scalar bosons, ghosts, gluons and electroweak gauge bosons, respectively.

number of independent degrees of freedom.

In Table 2 we list all Green's functions, which we have considered in the course of the calculations performed in this paper, and the number of generated Feynman amplitudes up to three loops. We used the following notation for the fields: B and W_i denote the gauge bosons, c_x refers to the ghost fields and Φ_i^0 and $\Phi_i^{\pm}$ ($i = 1, 2$) are the neutral and charged components of the scalar doublets. In Fig. 2 we show typical Feynman diagrams

contributing to the individual Green's functions.

Due to Ward identities there are various choices for each gauge coupling to obtain Z_{α_i}:

$$
\begin{aligned}
Z_{\alpha_1} &= \frac{1}{Z_{BB}} = \frac{(Z_{f_L \bar{f}_L B})^2}{Z_{BB} Z_L^f Z_L^f} = \dots, \\
Z_{\alpha_2} &= \frac{(Z_{c_{W_1} \bar{c}_{W_2} W_3})^2}{Z_{W_3 W_3}(Z_{c_{W_3} \bar{c}_{W_3}})^2} = \frac{(Z_{W_1 W_2 W_3})^2}{(Z_{W_3 W_3})^3} = \frac{(Z_{f_L \bar{f}_L W_3})^2}{Z_{W_3 W_3} Z_L^f Z_L^f} \\
&= \frac{(Z_{\Phi_1^+ \Phi_1^- W_3})^2}{Z_{W_3 W_3}(Z_{\Phi_1^+ \Phi_1^-})^2} = \frac{(Z_{\Phi_1^0 \Phi_1^0 W_3})^2}{Z_{W_3 W_3}(Z_{\Phi_1^0 \Phi_1^0})^2} = \dots, \\
Z_{\alpha_3} &= \frac{(Z_{c_g \bar{c}_g g})^2}{Z_{gg}(Z_{c_g \bar{c}_g})^2} = \frac{(Z_{ggg})^2}{(Z_{gg})^3} = \frac{(Z_{f_L \bar{f}_L g})^2}{Z_{gg} Z_L^f Z_L^f} = \dots,
\end{aligned}
\tag{25}
$$

where we have used $Z_{c_{W_1} \bar{c}_{W_1}} = Z_{c_{W_2} \bar{c}_{W_2}} = Z_{c_{W_3} \bar{c}_{W_3}}$ and $Z_{W_1 W_1} = Z_{W_2 W_2} = Z_{W_3 W_3}$. Here Z_L^f, Z_R^f with[3] $f = u, d, l$ stand for the wave functions renormalization of the left- and right-handed fermion fields. Their explicit definition will be introduced in the next section.

The lowest number of Feynman diagrams are generated for the Green's functions involving ghosts. Thus, our default choice for the computation of the gauge coupling renormalization constants are the gauge boson-ghost vertices and the corresponding two-point functions. Other vertices have been considered to have powerful cross checks. Due to the Ward identity the renormalization constant for α_1 is given by the inverse renormalization constant of the $U(1)$ gauge boson propagator. We have performed an explicit calculation of Z_{BB}, $Z_{c_{W_1} \bar{c}_{W_2} W_3}$, $Z_{W_3 W_3}$, $Z_{c_{W_3} \bar{c}_{W_3}}$, $Z_{u_L \bar{u}_L W_3}$, $Z_L^u Z_L^u$, $Z_{\Phi_1^0 \Phi_1^0 W_3}$, $Z_{\Phi_1^0 \Phi_1^0}$, $Z_{c_g \bar{c}_g g}$, Z_{gg}, $Z_{c_g \bar{c}_g}$.

For the Yukawa matrices we are restricted to vertices which involve components of the scalar doublets as well as left- and right-handed fermion fields. The explicit definition of the Yukawa matrix renormalization constants will be postponed to the next section.

At the end of this section a comment concerning γ_5 is in order. For the computation of some of the Green's functions an odd number of γ_5 matrices is present in the traces. We have checked that it is sufficient to follow the prescription provided in Ref. [2] in the context of the SM. This means that a formal replacement of expressions like

$$
\mathrm{Tr}\left(\gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \gamma_5\right) = -4\mathrm{i}\tilde{\epsilon}^{\mu\nu\rho\sigma} + \mathcal{O}(\epsilon) .
\tag{26}
$$

is applied, where $\tilde{\epsilon}^{\mu\nu\rho\sigma}$ is antisymmetric in all indices. In practice the product of two such objects occurs, where all indices are contracted, which we replace by

$$
\tilde{\epsilon}^{\mu\nu\rho\sigma} \tilde{\epsilon}_{\mu'\nu'\rho'\sigma'} = g^{[\mu}_{[\mu'} g^\nu_{\nu'} g^\rho_{\rho'} g^{\sigma]}_{\sigma']} .
\tag{27}
$$

The square brackets denote complete antisymmetrization. This leads to the correct result in the limit $d \to 4$. We have checked explicitly that the ambiguity of $\mathcal{O}(\epsilon)$ in Eq. (26) is multiplied by at most simple poles in ϵ and therefore does not lead to ambiguous renormalization constants and beta functions.

---

[3]In the case of Z_{α_3} we have $f = u, d$.

4 $\overline{\text{MS}}$ renormalization of the general 2HDM

4.1 Renormalization constants

For the computation of the renormalization constants for fields, couplings and vertices we follow the procedure described in Ref. [41]. However, since we consider general Yukawa couplings which are non-diagonal both in flavour as well as in doublet space, several modifications have to be applied, in particular for the calculation of the fermion and scalar wave function renormalization constants, and the renormalization constants for the Yukawa matrices. These issues are discussed in this section.

The renormalized inverse fermion propagator can be written as

$$S_F^{-1}(p) = \not{p} \left[P_L \left(\sqrt{Z_L^f} \right)^\dagger (1 + \Sigma_L(p^2)) \sqrt{Z_L^f} + P_R \left(\sqrt{Z_R^f} \right)^\dagger (1 + \Sigma_R(p^2)) \sqrt{Z_R^f} \right] , \quad (28)$$

where $P_{L/R} = (1 \mp \gamma_5)/2$, $\Sigma_{L/R}$ are the left- and right-handed parts of the fermion self energy and $Z_{L/R}^f$ are the renormalization constants for the left- and right-handed fermion fields. Both $\Sigma_{L/R}$ and $Z_{L/R}^f$ are matrices in flavour space where flavour indices have been suppressed. The index $f \in \{u, d, l\}$ indicates whether the up-, down- or lepton matrix shall be considered.

The renormalized two-point function of the scalar fields can be written as

$$\Pi^{\text{ren}}(p^2) = \left(\sqrt{Z^\Phi} \right)^\dagger \Pi(p^2) \sqrt{Z^\Phi} , \quad (29)$$

where the wave function renormalization constant Z^Φ and $\Pi(p^2)$ are matrices in doublet space. The corresponding indices have been suppressed. In $\mathbb{Z}_2$-symmetric models Z^Φ has to be diagonal, which we have checked up to three-loop level.

From Eqs. (28) and (29) the following relations can be derived:

$$\begin{aligned}
Z_L^f &= 1 - K_\epsilon \left[\left(\sqrt{Z_L^f} \right)^\dagger (1 + \Sigma_L(p^2)) \sqrt{Z_L^f} \right] , \\
Z_R^f &= 1 - K_\epsilon \left[\left(\sqrt{Z_R^f} \right)^\dagger (1 + \Sigma_R(p^2)) \sqrt{Z_R^f} \right] , \\
Z^\Phi &= 1 - K_\epsilon \left[\left(\sqrt{Z^\Phi} \right)^\dagger \Sigma(p^2) \sqrt{Z^\Phi} \right] .
\end{aligned} \quad (30)$$

The operator K_ϵ extracts the poles in ϵ. Solving these equations recursively allows to determine the corresponding renormalization constants. Let us stress at this point that from the equations above we can compute only the hermitian parts of the renormalization matrices Z_L^f, Z_R^f and Z^Φ. In the SM the anti-hermitian parts of the quark wave functions

renormalizations are related to the renormalization of the CKM matrix [42–44]. In the next section we will also introduce anti-hermitian contributions to the renormalization matrices defined above. However, in our case, they should not be identified with the renormalization of any physical quantity.

Let us in a next step use this information to obtain formulae which allow to compute the renormalization constants for the scalar-fermion vertices and the Yukawa couplings. The Yukawa vertex renormalization constants for a fermion of type f can be extracted from

$$\sum_{\beta} \sum_{b=1}^{2} Z_{ab,\alpha\beta}^{ff\Phi} Y_{b,\beta\alpha'}^{f} = Y_{a,\alpha\alpha'}^{f} - K_{\epsilon} \left[\sum_{\beta,\gamma} \sum_{b=1}^{2} \left(\sqrt{Z_L^f}_{\alpha\beta} \right)^{\dagger} \sqrt{Z^\Phi}_{ab} \Gamma(p,0)_{b,\beta\gamma} \sqrt{Z_R^f}_{\gamma\alpha'} \right] , \quad (31)$$

where for convenience the flavour (α, β, γ) and the doublet (a, b) indices are shown explicitly. The sums over β and γ run over all down-(up-)type fermions in case α is a down-(up-)type fermion. Note that in Eq. (31) $\Gamma(p,0)_{b,\beta\gamma}$ is the vertex function where one of the external momenta is set to zero and the external fields are Φ_b and fermions with flavour β and γ. Furthermore, the Yukawa coupling in the tree-level contribution of $\Gamma(p,0)_{b,\beta\gamma}$ is not renormalized.

Once $\sum_{\beta} \sum_{b=1}^{2} Z_{ab,\alpha\beta}^{ff\Phi} Y_{b,\beta\alpha'}^{f}$ is obtained from Eq. (31) the Yukawa matrix renormalization constants (ΔY_a^f) can be computed from

$$\sum_{\beta} \sum_{b=1}^{2} Z_{ab,\alpha\beta}^{ff\Phi} Y_{b,\beta\alpha'}^{f} = \sum_{\beta,\gamma} \sum_{b=1}^{2} \left(\sqrt{Z_L^f}_{\alpha\beta} \right)^{\dagger} \sqrt{Z^\Phi}_{ab} (Y_b^f + \Delta Y_b^f)_{\beta\gamma} \sqrt{Z_R^f}_{\gamma\alpha'} . \quad (32)$$

This equation has to be solved iteratively for $(Y_a^f + \Delta Y_a^f)$.

4.2   Invariants in the quark sector

The renormalization constants introduced in Eq. (30) are used to derive the corresponding anomalous dimensions. Note, however, that the anomalous dimensions might contain poles in ϵ. This is not surprising, since in the case of general Yukawa matrices we do not take into account the invariance of the theory under unitary rotations like those given in Eq. (3). In other words, from the 72 parameters[4] of the Yukawa sector of the general 2HDM 30 can be eliminated using flavour transformations [45][5]. In contrast to the case of Lagrangian parameters, the beta functions of the flavour invariants (cf. Eq. (18)) are finite, because the flavour symmetry relations are by construction taken into account in such quantities.

We also want to remark that the gauge couplings are trivially invariant under unitary flavour transformations and the corresponding beta functions do not suffer from uncanceled singularities. On the other hand, in analogy to the Yukawa matrices, we expect

---

[4]4 complex 3×3 matrices with 18 parameters each.
[5]The flavour symmetry group $[U(3)]^3 \otimes U(2)$ is broken by the Yukawa sector to $U(1)$, leading to 30 broken generators.

that in the case of the quartic couplings of the scalar potential only certain combinations of them have finite beta functions.

In the SM and in $\mathbb{Z}_2$-symmetric 2HDMs there are eleven flavour invariants in the quark sector as has been discussed in Section 2. From them the six quark masses, three CKM mixing angles, and the cosine and the sign of the CP-violating phase can be derived. Their behaviour under renormalization group evolution has been studied up to two loops, for example, in Ref. [25]. We have extended the analysis and checked by an explicit calculation that all eleven invariants in Eq. (18) of the SM and $\mathbb{Z}_2$-symmetric 2HDMs have finite anomalous dimensions at three loops. From the three-loop anomalous dimensions of the eleven invariants mentioned above one can derive the beta functions for the physical couplings and the CKM mixing angles to the same order.

As already mentioned in Section 2, we have not classified all flavour invariants in the general 2HDM. However, an explicit calculation for the invariants

$$\mathrm{Tr}\left(Y_a^u Y_a^{u\dagger}\right), \mathrm{Tr}\left(Y_a^d Y_a^{d\dagger}\right), \mathrm{Tr}\left(Y_a^u Y_b^{u\dagger} Y_b^u Y_a^{u\dagger}\right), \mathrm{Tr}\left(Y_a^u Y_a^{u\dagger} Y_b^u Y_b^{u\dagger}\right),$$

$$\mathrm{Tr}\left(Y_a^d Y_b^{d\dagger} Y_b^d Y_a^{d\dagger}\right), \mathrm{Tr}\left(Y_a^d Y_a^{d\dagger} Y_b^d Y_b^{d\dagger}\right), \mathrm{Tr}\left(Y_a^u Y_a^{u\dagger} Y_b^d Y_b^{d\dagger}\right), \mathrm{Tr}\left(Y_a^u Y_b^{u\dagger} Y_a^d Y_b^{d\dagger}\right),$$

$$\mathrm{Tr}\left(Y_a^u Y_a^{u\dagger}\right)\mathrm{Tr}\left(Y_b^u Y_a^{u\dagger}\right), \mathrm{Tr}\left(Y_a^d Y_b^{d\dagger}\right)\mathrm{Tr}\left(Y_b^d Y_a^{d\dagger}\right), \mathrm{Tr}\left(Y_a^u Y_b^{u\dagger}\right)\mathrm{Tr}\left(Y_a^d Y_b^{d\dagger}\right), \qquad (33)$$

where we sum over a and b and the trace is taken over the fermionic indices, shows that all poles cancel.

4.3   Invariants for a simplified model

In this Subsection we consider a simplified version of the general 2HDM. Explicitly, we study the case where the Yukawa interactions for the first and second generations are neglected. As a consequence, the Yukawa matrices reduce to complex numbers, parameterizing the Yukawa couplings for the t and b quarks and only scalar flavour symmetries occur. Following Ref. [45], one observes that from the eight parameters[6] in the Yukawa sector $(n^2 - 1) \overset{n=2}{=} 3$ can be rotated away. We also notice that the up- and down-type Yukawa couplings transform as vectors under unitary rotations of the scalar fields, see Eq. (4) where U_Q and $U_{u,d}$ are replaced by the identity matrix for this simplified model. We thus rotate the scalar fields with the following matrix

$$U_\Phi = \frac{1}{\sqrt{y_1^t y_1^{t*} + y_2^t y_2^{t*}}} \begin{pmatrix} y_1^{t*} & y_2^{t*} \\ -y_2^t & y_1^t \end{pmatrix}. \qquad (34)$$

Under this transformation the scalar fields change to

$$\Phi_1' = \frac{\delta_{ij} y_i^{t*}}{\sqrt{I_t}} \Phi_j,$$

---

[6]We have $y_i^f \in \mathbb{C}$ with $f = u, d$ and $i = 1, 2$.

$$\Phi'_2 \;\; = \;\; \frac{\varepsilon_{ij} y_i^t}{\sqrt{I_t}} \Phi_j \tag{35}$$

with $I_t = \delta_{ij} y_i^t y_j^{t*}$. δ_{ab} and ε_{ab} denote the Kronecker delta and Levi-Civita tensor, respectively, and the sum over the repeated indices $i, j = 1, 2$ is assumed. Furthermore, the Yukawa couplings transform as

$$\begin{aligned}
y_1^{t\prime} &= \sqrt{\delta_{ij} y_i^t y_j^{t*}} \;=\; \sqrt{I_t}\,, & y_2^{t\prime} &= 0\,, \\
y_1^{b\prime} &= \frac{\delta_{ij} y_i^t y_j^b}{\sqrt{I_t}}\,, & y_2^{b\prime} &= \frac{\varepsilon_{ij} y_i^b y_j^{t*}}{\sqrt{I_t}}\,.
\end{aligned} \tag{36}$$

Taking into account the tensorial properties of δ_{ab} and ε_{ab} and the transformations of the Yukawa couplings under unitary rotations of the scalar fields, one can easily prove that both the rotated fields and couplings are actually flavour invariants. In other words, in the new basis the Lagrangian parameters are expressed through flavour invariants and are therefore directly related to physical quantities.

An explicit calculation shows that the anomalous dimensions of the new fields Φ'_a with $a = 1, 2$ and the beta functions of the new couplings $y_1^{t\prime}$, $y_1^{b\prime}$ and $y_2^{b\prime}$ are finite through three loops. This is not the case for the original basis, where the Yukawa sector contains too many parameters. The new basis makes use of the flavour symmetries and gets rid of one of the up-type Yukawa couplings, the other one is rendered real. It is also important to notice that the relation $y_2^{t\prime} = 0$ is stable under renormalization. To verify this statement, we checked through three loops that the beta functions of the three Yukawa couplings obtained after the rotation to the new basis can be expressed only in terms of couplings present in this basis. At this stage, also the scalar quartic couplings have to be transformed according to Eqs. (8). This shows that the set of couplings in the new basis is complete. Even for this simplified model the explicit three-loop results are quite lengthy. Thus, in Section 6 we only present results for $\beta_{y_1^{t\prime}}$.

4.4 Poles in anomalous dimensions

In this Subsection we describe a practical method, which allows to use the beta functions and anomalous dimensions for a general 2HDM, although they develop poles in the first place. A transformation to physical observables, which, as mentioned above, becomes quite involved, is not necessary. We follow Ref. [6], where this issue has been discussed for the case of the SM. It is argued that the poles can be eliminated by choosing the square roots of the renormalization constants to be non-hermitian. We define

$$\sqrt{Z} = \sqrt{Z}_H \sqrt{Z}_U \,, \tag{37}$$

where Z is any of the renormalization constants introduced in Eq. (30). The subscripts H and U in Eq. (37) denote the hermitian and unitary parts.

In order to obtain $Y^u + \Delta Y^u$ one has to invert Eq. (32). This can be done by either choosing hermitian square roots or by allowing for additional unitary factors which leads to the following relation

$$Y'^u_a + \Delta Y'^u_a = \sqrt{Z_{L_U}} \left(Y^u_b + \Delta Y^u_b\right) \left(\sqrt{Z_R}\right)^\dagger_U \sqrt{Z_{\Phi_U,ba}} \,, \tag{38}$$

where the $Y^u + \Delta Y^u$ is calculated with hermitian square roots. This equation resembles the transformation in Eq. (4) and therefore a choice of the unitary part of the square root of the Z factors can be interpreted as a certain choice of basis.

$\sqrt{Z_H}$ is fixed by the poles of the corresponding two point functions in Eq. (30) and can be used to obtain the hermitian part of the corresponding anomalous dimensions, i.e., the combination $\gamma + \gamma^\dagger$. For the left- and right-handed fermion fields and the scalar fields considered in Eq. (30) we observe that $\gamma + \gamma^\dagger$ is finite whereas the individual terms are not.

Note, however, that $\sqrt{Z_U}$ is an arbitrary unitary matrix which can be chosen such that γ is finite. This choice is not unique and it is possible to also influence the finite parts of the anomalous dimensions (and in general the beta functions) this way. We will postpone the discussion of this apparent ambiguity and its physical significance to Subsection 4.5 and concentrate in the following on the discussion of the left-handed quark fields.

At one-loop order there is no possibility to construct $\sqrt{Z^Q_L}_U \neq \mathbb{I}$ and therefore $\sqrt{Z^Q_L}$ is purely hermitian. At two-loop order there is one unitary combination of Yukawa matrices

$$\sqrt{Z^Q_L}_U = \mathbb{I} + \left(\frac{a}{\epsilon^2} + \frac{b}{\epsilon}\right) \left[Y^u Y^{u\dagger}, Y^d Y^{d\dagger}\right] \,, \tag{39}$$

where a and b are arbitrary constants. A nonzero value for b enters into the finite parts of the left-handed quark field anomalous dimension and therefore into the beta functions for Y^u and Y^d, contributing to the mentioned ambiguity (see below Subsection 4.5).

One can choose a nonzero value for a to cancel possible ϵ poles in the non-hermitian part of the two-loop anomalous dimension. However, such poles can not appear as can be seen by the following arguments: For the anomalous dimensions we schematically write

$$\gamma = -\sqrt{Z^Q_L}^{-1} \mu \frac{\mathrm{d}}{\mathrm{d}\mu} \sqrt{Z^Q_L} \,,$$
$$\gamma^\dagger = -\left(\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \sqrt{Z^Q_L}^\dagger\right) \sqrt{Z^Q_L}^{\dagger-1} \,, \tag{40}$$

where the second equation simplifies to

$$\gamma^\dagger = -\left(\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \sqrt{Z^Q_L}\right) \sqrt{Z^Q_L}^{-1} \tag{41}$$

in the case hermitian square roots are chosen. Thus, the anomalous dimension is hermitian (and finite) if the commutator

$$\left[\left(\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \sqrt{Z_L^Q} \right), \sqrt{Z_L^Q}^{-1} \right] = 0 \tag{42}$$

is satisfied. At two-loop order only the contribution where both terms in Eq. (42) receive one-loop contributions involving two Yukawa matrices could possibly lead to a nonvanishing commutator of the form

$$\left[Y^u Y^{u\dagger}, Y^d Y^{d\dagger} \right] \ . \tag{43}$$

However, an explicit calculation in the general 2HDM model shows that $Y^u Y^{u\dagger}$ and $Y^d Y^{d\dagger}$ appear with the same coefficients in the renormalization constant and thus the commutator is zero and no non-trivial factor $\sqrt{Z_L^Q}_U$ is needed.

At three loops we have $\gamma \neq \gamma^\dagger$ in case hermitian square root factors are chosen. For example, there are contributions to Z_L^Q involving $Y^u Y^{u\dagger}$ or $Y^d Y^{d\dagger}$, however, with different prefactors for up- and down-type quarks due to the presence of hyper-charge contributions. This leads to a non-vanishing commutator in Eq. (42). Thus, the necessity to choose a nontrivial factor $\sqrt{Z_L^Q}_U$ arises from three loops.

Similar arguments hold for the scalar and right-handed quark fields.

4.5 Ambiguities in the Yukawa matrix beta function

The possibility to introduce $\sqrt{Z}_U \neq \mathbb{I}$ introduces an ambiguity in the definition of the renormalization constants, anomalous dimensions and beta functions. Nevertheless, let us stress that this statement only holds for the unphysical parameters, e.g. the Yukawa matrices. Once we construct flavour invariants the unitary roots cancel and their anomalous dimensions are finite and unambiguous. Consequently, the anomalous dimensions of the physical quantities derived from them are finite and unambiguous, as expected.

We verified the cancellation of the unitary roots and consequently the poles in the beta functions for all eleven invariants of the quark sector of $\mathbb{Z}_2$-symmetric 2HDMs. Furthermore, we checked the cancellation in the general 2HDM for the invariants introduced in Section 2 as well as further invariants entering the gauge coupling beta functions, which we will present in the next section (see Eqs. (48) and (49)).

In addition, we also performed numerical checks by computing the Yukawa matrices in $\mathbb{Z}_2$-symmetric 2HDMs at a low scale and run them up to 10^{16} GeV for different choices of $\sqrt{Z}_U$, modifying the finite part of the beta functions. While the Yukawa matrices themselves differ at the high scale, depending on the choice of $\sqrt{Z}_U$, their eigenvalues do not, showing again that the ambiguity does not affect physical quantities.

5 Results for the gauge coupling beta functions

In this section we present the analytical results for the gauge coupling beta functions of a general 2HDM. We notice that both the Yukawa matrices and the self couplings occur in the gauge beta functions only through flavour invariants[7], as expected.

We present the results keeping the full information contained in the Yukawa matrices and arrive at the following expressions for the beta functions

$$
\begin{aligned}
\beta_1 = & -\epsilon \frac{\alpha_1}{\pi} + \frac{\alpha_1^2}{(4\pi)^2}\left[\frac{16}{3}n_G + \frac{2}{5}n_D\right] \\
& + \frac{\alpha_1^2}{(4\pi)^3}\left[n_G\left(\frac{76\alpha_1}{15} + \frac{12\alpha_2}{5} + \frac{176\alpha_3}{15}\right) + n_D\left(\frac{18\alpha_1}{25} + \frac{18\alpha_2}{5}\right)\right. \\
& \left. - \frac{34}{5}\operatorname{Tr}(\hat{M}_u) - 2\operatorname{Tr}\hat{M}_d - 6\operatorname{Tr}\hat{M}_l\right] \\
& + \frac{\alpha_1^2}{(4\pi)^4}\left[n_G^2\left(-\frac{836\alpha_1^2}{135} - \frac{44\alpha_2^2}{15} - \frac{1936\alpha_3^2}{135}\right) + n_D^2\left(-\frac{147\alpha_1^2}{1000} - \frac{49\alpha_2^2}{40}\right)\right. \\
& + n_G n_D\left(-\frac{887\alpha_1^2}{450} - \frac{173\alpha_2^2}{30}\right) + n_D\left(\frac{783\alpha_1^2}{2000} + \frac{783\alpha_1\alpha_2}{200} + \frac{3499\alpha_2^2}{80}\right) \\
& + n_G\left(-\frac{101\alpha_1^2}{90} - \frac{7\alpha_1\alpha_2}{25} - \frac{548\alpha_1\alpha_3}{225} + \frac{101\alpha_2^2}{6} - \frac{4\alpha_2\alpha_3}{5} + \frac{1100\alpha_3^2}{9}\right) \\
& - \frac{2827\alpha_1}{200}\operatorname{Tr}(\hat{M}_u) - \frac{1267\alpha_1}{200}\operatorname{Tr}(\hat{M}_d) - \frac{2529\alpha_1}{200}\operatorname{Tr}(\hat{M}_l) - \frac{471\alpha_2}{8}\operatorname{Tr}(\hat{M}_u) \\
& - \frac{1311\alpha_2}{40}\operatorname{Tr}(\hat{M}_d) - \frac{1629\alpha_2}{40}\operatorname{Tr}(\hat{M}_l) - \frac{116\alpha_3}{5}\operatorname{Tr}(\hat{M}_u) - \frac{68\alpha_3}{5}\operatorname{Tr}(\hat{M}_d) \\
& + \frac{9\alpha_1}{25}\hat{\lambda}_{ij,ji} + \frac{18\alpha_1}{25}\hat{\lambda}_{ii,jj} + \frac{9\alpha_2}{5}\hat{\lambda}_{ij,ji} + \frac{213}{20}\operatorname{Tr}(\hat{M}_u^2) + \frac{81}{20}\operatorname{Tr}(\hat{M}_d^2) \\
& + \frac{3}{10}\operatorname{Tr}(\hat{M}_u\hat{M}_d) + \frac{63}{10}\operatorname{Tr}(\hat{M}_{uu}^{(2)}) + \frac{51}{10}\operatorname{Tr}(\hat{M}_{dd}^{(2)}) + \frac{6}{5}\operatorname{Tr}(\hat{M}_{ud}^{(2)}) \\
& + \frac{147}{20}\operatorname{Tr}(\hat{M}_l^2) + \frac{57}{10}\operatorname{Tr}(\hat{M}_{ll}^{(2)}) + \frac{303}{10}\hat{T}_{uu}^{(2)} + \frac{51}{10}\hat{T}_{dd}^{(2)} + \frac{177}{5}\hat{T}_{ud}^{(2)} + \frac{99}{10}\hat{T}_{ll}^{(2)} \\
& \left. + \frac{199}{5}\hat{T}_{ul}^{(2)} + \frac{157}{5}\hat{T}_{dl}^{(2)} - \frac{3}{5}\hat{\lambda}_{ij,kl}\hat{\lambda}_{ji,lk} - \frac{6}{5}\hat{\lambda}_{ij,kl}\hat{\lambda}_{li,jk}\right],
\end{aligned} \tag{44}
$$

---

[7]Some of them are identical to the invariants listed in Eq. (18).

$$\beta_2 = -\epsilon\frac{\alpha_2}{\pi} + \frac{\alpha_2^2}{(4\pi)^2}\left[-\frac{88}{3} + \frac{16}{3}n_G + \frac{2}{3}n_D\right]$$

$$+ \frac{\alpha_2^2}{(4\pi)^3}\left[-\frac{544\alpha_2}{3} + n_G\left(\frac{4\alpha_1}{5} + \frac{196\alpha_2}{3} + 16\alpha_3\right) + n_D\left(\frac{6\alpha_1}{5} + \frac{26\alpha_2}{3}\right)\right.$$

$$\left. - 6\operatorname{Tr}(\hat{M}_u + \hat{M}_d) - 2\operatorname{Tr}\hat{M}_l\right]$$

$$+ \frac{\alpha_2^2}{(4\pi)^4}\left[-\frac{45712\alpha_2^2}{27} + n_G^2\left(-\frac{44\alpha_1^2}{45} - \frac{1660\alpha_2^2}{27} - \frac{176\alpha_3^2}{9}\right) + n_D^2\left(-\frac{49\alpha_1^2}{200} - \frac{425\alpha_2^2}{216}\right)\right.$$

$$+ n_G n_D\left(-\frac{91\alpha_1^2}{50} - \frac{1121\alpha_2^2}{54}\right) + n_D\left(\frac{261\alpha_1^2}{400} + \frac{561\alpha_1\alpha_2}{40} + \frac{65131\alpha_2^2}{432}\right)$$

$$+ n_G\left(-\frac{7\alpha_1^2}{150} + \frac{13\alpha_1\alpha_2}{5} - \frac{4\alpha_1\alpha_3}{15} + \frac{52417\alpha_2^2}{54} + 52\alpha_2\alpha_3 + \frac{500\alpha_3^2}{3}\right)$$

$$- \frac{593\alpha_1}{40}\operatorname{Tr}(\hat{M}_u) - \frac{533\alpha_1}{40}\operatorname{Tr}(\hat{M}_d) - \frac{51\alpha_1}{8}\operatorname{Tr}(\hat{M}_l)$$

$$- \frac{729\alpha_2}{8}\operatorname{Tr}(\hat{M}_u + \hat{M}_d) - \frac{243\alpha_2}{8}\operatorname{Tr}(\hat{M}_l) - 28\alpha_3\operatorname{Tr}(\hat{M}_u + \hat{M}_d)$$

$$+ \frac{3\alpha_1}{5}\hat{\lambda}_{ij,ji} + \alpha_2\hat{\lambda}_{ij,ji} + 2\alpha_2\hat{\lambda}_{ii,jj} + \frac{15}{4}\operatorname{Tr}((\hat{M}_u + \hat{M}_d)^2)$$

$$+ \frac{21}{2}\operatorname{Tr}(\hat{M}_{uu}^{(2)} + \hat{M}_{dd}^{(2)}) + 6\operatorname{Tr}(\hat{M}_{ud}^{(2)}) + \frac{5}{4}\operatorname{Tr}(\hat{M}_l^2) + \frac{7}{2}\operatorname{Tr}(\hat{M}_{ll}^{(2)})$$

$$+ \frac{45}{2}(\hat{T}_{uu}^{(2)} + \hat{T}_{dd}^{(2)} + 2\hat{T}_{ud}^{(2)}) + \frac{5}{2}\hat{T}_{ll}^{(2)} + 15(\hat{T}_{ul}^{(2)} + \hat{T}_{dl}^{(2)})$$

$$\left. - \hat{\lambda}_{ij,kl}\hat{\lambda}_{ji,lk} - 2\hat{\lambda}_{ij,kl}\hat{\lambda}_{li,jk}\right], \tag{45}$$

and

$$\beta_3 = -\epsilon\frac{\alpha_3}{\pi} + \frac{\alpha_3^2}{(4\pi)^2}\left[-44 + \frac{16}{3}n_G\right]$$

$$+ \frac{\alpha_3^2}{(4\pi)^3}\left[-408\alpha_3 + n_G\left(\frac{22\alpha_1}{15} + 6\alpha_2 + \frac{304\alpha_3}{3}\right) - 8\operatorname{Tr}(\hat{M}_u + \hat{M}_d)\right]$$

$$+ \frac{\alpha_3^2}{(4\pi)^4}\left[-5714\alpha_3^2 + n_G^2\left(-\frac{242\alpha_1^2}{135} - \frac{22\alpha_2^2}{3} - \frac{2600\alpha_3^2}{27}\right) + n_G n_D\left(-\frac{253\alpha_1^2}{900} - \frac{23\alpha_2^2}{12}\right)\right.$$

$$+ n_G \Big(- \frac{137\alpha_1^2}{900} - \frac{\alpha_1\alpha_2}{10} + \frac{308\alpha_1\alpha_3}{45} + \frac{505\alpha_2^2}{12} + 28\alpha_2\alpha_3 + \frac{20132\alpha_3^2}{9} \Big)$$

$$- \frac{101\alpha_1}{10} \operatorname{Tr}(\hat{M}_u) - \frac{89\alpha_1}{10} \operatorname{Tr}(\hat{M}_d) - \frac{93\alpha_2}{2} \operatorname{Tr}(\hat{M}_u + \hat{M}_d)$$

$$- 160\alpha_3 \operatorname{Tr}(\hat{M}_u + \hat{M}_d) + 6 \operatorname{Tr}((\hat{M}_u + \hat{M}_d)^2) + 12 \operatorname{Tr}(\hat{M}_{uu}^{(2)} + \hat{M}_{dd}^{(2)} - 2\hat{M}_{ud}^{(2)})$$

$$+ 42(\hat{T}_{uu}^{(2)} + \hat{T}_{dd}^{(2)} + 2\hat{T}_{ud}^{(2)}) + 14(\hat{T}_{ul}^{(2)} + \hat{T}_{dl}^{(2)}) \bigg]. \tag{46}$$

In the above equations n_G denotes the number of fermion generations and n_D the number of scalar doublets. We sum over the indices i, j, k, l of the quartic couplings from 1 to n_D. The matrix M_l is defined by

$$M_l = Y_1^l Y_1^{l\dagger} + Y_2^l Y_2^{l\dagger} \tag{47}$$

in analogy to Eq. (17). Other combinations of Yukawa matrices are given by

$$M_{uu}^{(2)} = \sum_{i,j=1}^{n_D} Y_i^u Y_j^{u\dagger} Y_j^u Y_i^{u\dagger} \,,$$

$$M_{dd}^{(2)} = \sum_{i,j=1}^{n_D} Y_i^d Y_j^{d\dagger} Y_j^d Y_i^{d\dagger} \,,$$

$$M_{ll}^{(2)} = \sum_{i,j=1}^{n_D} Y_i^l Y_j^{l\dagger} Y_j^l Y_i^{l\dagger} \,,$$

$$M_{ud}^{(2)} = \sum_{i,j=1}^{n_D} Y_i^u Y_j^{u\dagger} Y_i^d Y_j^{d\dagger} \,, \tag{48}$$

as well as

$$T_{ll}^{(2)} = \sum_{i,j=1}^{n_D} \operatorname{Tr}(Y_i^l Y_j^{l\dagger}) \operatorname{Tr}(Y_j^l Y_i^{l\dagger}) \,,$$

$$T_{ud}^{(2)} = \sum_{i,j=1}^{n_D} \operatorname{Tr}(Y_i^u Y_j^{u\dagger}) \operatorname{Tr}(Y_i^d Y_j^{d\dagger}) \,,$$

$$T_{ul}^{(2)} = \sum_{i,j=1}^{n_D} \operatorname{Tr}(Y_i^u Y_j^{u\dagger}) \operatorname{Tr}(Y_i^l Y_j^{l\dagger}) \,,$$

$$T_{dl}^{(2)} = \sum_{i,j=1}^{n_D} \operatorname{Tr}(Y_i^d Y_j^{d\dagger}) \operatorname{Tr}(Y_j^l Y_i^{l\dagger}) \,. \tag{49}$$

which are defined in analogy to Eqs. (19) and (20). We rescaled the Yukawa matrices in the above results such that $\hat{M}_f = M_f/(4\pi)$, $\hat{T}^{(2)}_{ff'} = T^{(2)}_{ff'}/(4\pi)^2$ and $\hat{M}^{(2)}_{ff'} = M^{(2)}_{ff'}/(4\pi)^2$. The results for the beta functions and the corresponding renormalization constants can be obtained in computer readable form [30].

We have performed a number of cross checks on the correctness of our result. Among them is the independence on the three gauge parameters. Furthermore, we can easily take the SM limit by setting $n_D = 1$, $Y^f_2 = 0$ and $\lambda_{ij,kl} = \lambda$ and find agreement with Refs. [1–3]. We also agree with the findings of Ref. [19] where results for a general theory based on a simple gauge group are presented.[8]

A comment on the validity of our results for $n_D \geq 3$ is in order. At three-loop order, all diagrams containing at least one internal gauge boson or a closed fermion loop can only receive contributions from up to two different scalar doublets. However, diagrams containing two quartic couplings can get contributions from more than two doublets. Therefore, all contributions to the three-loop beta functions are also valid for $n_D \geq 3$ apart from those containing two quartic couplings.

6   Results for the Yukawa coupling beta functions

As discussed in Section 4 the Yukawa matrix beta functions themselves are ambiguous and one should either work in a proper basis or only consider invariants of the Yukawa sector. In general the expressions are quite lengthy at three loops. Thus, we restrict ourselves to the beta function in the simplified model discussed in Section 4.3. For simplicity we drop the primes introduced in Eq. (36) and write $y^t \equiv y^t_1$ since $\beta_{y^t_2} = 0$. We obtain

$$
\begin{aligned}
\beta_{y^t} = {}& -\epsilon \frac{y^t}{2} + \frac{y^t}{4\pi}\left[-\frac{17\alpha_1}{40} - \frac{9\alpha_2}{8} - 4\alpha_3 + \frac{9\hat{y}^{t2}}{4} + \frac{3\left|\hat{y}^b_1\right|^2}{4} + \frac{\left|\hat{y}^b_2\right|^2}{4} \right] \\
& + \frac{y^t}{(4\pi)^2}\left[\frac{107\alpha_1^2}{1200} - \frac{9\alpha_1\alpha_2}{40} + \frac{19\alpha_1\alpha_3}{30} - \frac{33\alpha_2^2}{8} + \frac{9\alpha_2\alpha_3}{2} - \frac{202\alpha_3^2}{3} + n_G\left(\frac{29\alpha_1^2}{90} + \frac{\alpha_2^2}{2}\right.\right. \\
& + \left.\frac{40\alpha_3^2}{9}\right) + \alpha_1\left(\frac{393\hat{y}^{t2}}{160} + \frac{7\left|\hat{y}^b_1\right|^2}{160} - \frac{41\left|\hat{y}^b_2\right|^2}{480}\right) + \alpha_2\left(\frac{225\hat{y}^{t2}}{32} + \frac{99\left|\hat{y}^b_1\right|^2}{32}\right. \\
& + \left.\frac{33\left|\hat{y}^b_2\right|^2}{32}\right) + \alpha_3\left(18\hat{y}^{t2} + 2\left|\hat{y}^b_1\right|^2 + \frac{8\left|\hat{y}^b_2\right|^2}{3}\right) - 6\hat{y}^{t4} - \frac{11\hat{y}^{t2}\left|\hat{y}^b_1\right|^2}{8} - \frac{5\hat{y}^{t2}\left|\hat{y}^b_2\right|^2}{4} \\
& - \frac{\left|\hat{y}^b_1\right|^4}{8} - \frac{11\left|\hat{y}^b_1\right|^2\left|\hat{y}^b_2\right|^2}{8} - \frac{5\left|\hat{y}^b_2\right|^4}{4} + 3\hat{\lambda}^2_{11,11} + \frac{\hat{\lambda}^2_{11,22}}{2} + \frac{\hat{\lambda}^2_{12,21}}{2} + \frac{\hat{\lambda}_{11,22}\hat{\lambda}_{12,21}}{2} \\
& + 3\hat{\lambda}_{12,12}\hat{\lambda}_{21,21} + \frac{9\hat{\lambda}_{11,12}\hat{\lambda}_{11,21}}{4} + \frac{3\hat{\lambda}_{12,22}\hat{\lambda}_{21,22}}{4} - 6\hat{y}^{t2}\hat{\lambda}_{11,11} - \left|\hat{y}^b_2\right|^2\hat{\lambda}_{11,22}
\end{aligned}
$$

---

[8]In this context one has to take into account the comments presented at the end of Section IV of Ref. [2].

$$+ \left| \hat{y}_2^b \right|^2 \hat{\lambda}_{12,21} \Bigg]$$

$$+ \frac{y^t}{(4\pi)^3} \Bigg[\frac{3701\alpha_1^3}{6000} + \frac{777\alpha_1^2\alpha_2}{400} - \frac{859\alpha_1^2\alpha_3}{400} + \frac{687\alpha_1\alpha_2^2}{320} - \frac{321\alpha_1\alpha_2\alpha_3}{40} - \frac{127\alpha_1\alpha_3^2}{120}$$

$$- \frac{699\alpha_2^3}{64} + \frac{501\alpha_2^2\alpha_3}{16} + \frac{531\alpha_2\alpha_3^2}{8} - 1249\alpha_3^3 + \zeta_3\Big(-\frac{153\alpha_1^3}{1000} - \frac{153\alpha_1^2\alpha_2}{200}$$

$$- \frac{27\alpha_1\alpha_2^2}{40} + \frac{45\alpha_2^3}{8} \Big) + n_G\Big(\frac{56861\alpha_1^3}{21600} + \frac{241\alpha_1^2\alpha_2}{800} + \frac{5281\alpha_1^2\alpha_3}{1800} - \frac{9\alpha_1\alpha_2^2}{160}$$

$$+ \frac{44\alpha_1\alpha_3^2}{9} - \frac{99\alpha_2^3}{32} + \frac{57\alpha_2^2\alpha_3}{8} + 19\alpha_2\alpha_3^2 + \frac{4432\alpha_3^3}{27} \Big) + n_G\zeta_3\Big(-\frac{323\alpha_1^3}{150}$$

$$- \frac{51\alpha_1^2\alpha_2}{50} - \frac{374\alpha_1^2\alpha_3}{75} - \frac{9\alpha_1\alpha_2^2}{10} - \frac{88\alpha_1\alpha_3^2}{15} + \frac{45\alpha_2^3}{2} - 18\alpha_2^2\alpha_3 - 24\alpha_2\alpha_3^2$$

$$+ \frac{320\alpha_3^3}{3} \Big) + n_G^2\Big(\frac{73\alpha_1^3}{81} + \frac{25\alpha_2^3}{9} + \frac{560\alpha_3^3}{81} \Big) + \alpha_1^2\Big(-\frac{69721\hat{y}^{t2}}{38400} - \frac{7159\left|\hat{y}_1^b\right|^2}{7680}$$

$$- \frac{101419\left|\hat{y}_2^b\right|^2}{115200} - \frac{1089\hat{\lambda}_{11,11}}{800} - \frac{363\hat{\lambda}_{11,22}}{800} - \frac{363\hat{\lambda}_{12,21}}{1600} + \zeta_3\Big(-\frac{93\hat{y}^{t2}}{400}$$

$$- \frac{199\left|\hat{y}_1^b\right|^2}{400} + \frac{11\left|\hat{y}_2^b\right|^2}{400} \Big) + n_G\Big(-\frac{115\hat{y}^{t2}}{32} - \frac{23\left|\hat{y}_1^b\right|^2}{480} - \frac{17\left|\hat{y}_2^b\right|^2}{96} \Big) \Big)$$

$$+ \alpha_1\alpha_2\Big(\frac{8097\hat{y}^{t2}}{1280} + \frac{747\left|\hat{y}_1^b\right|^2}{256} + \frac{773\left|\hat{y}_2^b\right|^2}{1280} + \frac{117\hat{\lambda}_{11,11}}{80} + \frac{117\hat{\lambda}_{12,21}}{160}$$

$$+ \zeta_3\Big(\frac{369\hat{y}^{t2}}{40} + \frac{27\left|\hat{y}_1^b\right|^2}{20} + \frac{9\left|\hat{y}_2^b\right|^2}{20} \Big) \Big) + \alpha_1\alpha_3\Big(-\frac{63\hat{y}^{t2}}{5} - \frac{457\left|\hat{y}_1^b\right|^2}{60}$$

$$- \frac{259\left|\hat{y}_2^b\right|^2}{72} + \zeta_3\Big(18\hat{y}^{t2} - \frac{14\left|\hat{y}_1^b\right|^2}{5} + \frac{16\left|\hat{y}_2^b\right|^2}{5} \Big) \Big) + \alpha_2^2\Big(\frac{47649\hat{y}^{t2}}{512}$$

$$+ \frac{13155\left|\hat{y}_1^b\right|^2}{512} + \frac{4329\left|\hat{y}_2^b\right|^2}{512} - \frac{171\hat{\lambda}_{11,11}}{32} - \frac{57\hat{\lambda}_{11,22}}{32} - \frac{57\hat{\lambda}_{12,21}}{64}$$

$$+ \zeta_3\Big(-\frac{729\hat{y}^{t2}}{16} - \frac{225\left|\hat{y}_1^b\right|^2}{32} - \frac{99\left|\hat{y}_2^b\right|^2}{32} \Big) + n_G\Big(-\frac{351\hat{y}^{t2}}{32} - \frac{69\left|\hat{y}_1^b\right|^2}{16}$$

$$- \frac{63\left|\hat{y}_2^b\right|^2}{16} \Big) \Big) + \alpha_2\alpha_3\Big(-84\hat{y}^{t2} - \frac{27\left|\hat{y}_1^b\right|^2}{4} + \frac{37\left|\hat{y}_2^b\right|^2}{8} + \zeta_3\Big(90\hat{y}^{t2} - 54\left|\hat{y}_1^b\right|^2 \Big) \Big)$$

$$+ \alpha_3^2\Big(\frac{4799\hat{y}^{t2}}{12} - \frac{277\left|\hat{y}_1^b\right|^2}{4} + \frac{2227\left|\hat{y}_2^b\right|^2}{36} + \zeta_3\Big(-114\hat{y}^{t2} - 22\left|\hat{y}_1^b\right|^2 - 34\left|\hat{y}_2^b\right|^2 \Big)$$

$$+ n_G\Big(-27\hat{y}^{t2} - \frac{7\left|\hat{y}_1^b\right|^2}{3} - \frac{11\left|\hat{y}_2^b\right|^2}{3} \Big) \Big) + \alpha_1\Big(-\frac{2437\hat{y}^{t4}}{160} - \frac{1383\hat{y}^{t2}\left|\hat{y}_1^b\right|^2}{320}$$

$$- \frac{697\hat{y}^{t2}\left|\hat{y}_2^b\right|^2}{480} - \frac{959\left|\hat{y}_1^b\right|^4}{320} - \frac{1133\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2}{960} + \frac{109\left|\hat{y}_2^b\right|^4}{60} + \zeta_3\Big(\frac{\hat{y}^{t2}\left|\hat{y}_1^b\right|^2}{4}$$

$$+ \frac{3\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2}{4} + \frac{19\left|\hat{y}_1^b\right|^4}{20} - \frac{2\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2}{5} - \frac{27\left|\hat{y}_2^b\right|^4}{20}\Big) - \frac{127\hat{y}^{t\,2}\hat{\lambda}_{11,11}}{20}$$

$$- \frac{139\left|\hat{y}_2^b\right|^2\hat{\lambda}_{11,22}}{120} + \frac{139\left|\hat{y}_2^b\right|^2\hat{\lambda}_{12,21}}{120} + \frac{9\hat{\lambda}_{11,11}^2}{2} + \frac{3\hat{\lambda}_{11,22}^2}{4} + \frac{3\hat{\lambda}_{12,21}^2}{4}$$

$$+ \frac{3\hat{\lambda}_{11,22}\hat{\lambda}_{12,21}}{4} + \frac{9\hat{\lambda}_{12,12}\hat{\lambda}_{21,21}}{2} + \frac{27\hat{\lambda}_{11,12}\hat{\lambda}_{11,21}}{8} + \frac{9\hat{\lambda}_{12,22}\hat{\lambda}_{21,22}}{8}\Big)$$

$$+ \alpha_2\Big(-\frac{1593\hat{y}^{t\,4}}{32} - \frac{2307\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^2}{64} - \frac{141\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2}{32} - \frac{2283\left|\hat{y}_1^b\right|^4}{64} - \frac{2763\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2}{64}$$

$$- \frac{15\left|\hat{y}_2^b\right|^4}{2} + \zeta_3\Big(-\frac{9\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^2}{4} - \frac{9\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2}{4} + \frac{63\left|\hat{y}_1^b\right|^4}{4} + 18\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2 + \frac{9\left|\hat{y}_2^b\right|^4}{4}\Big)$$

$$- \frac{135\hat{y}^{t\,2}\hat{\lambda}_{11,11}}{4} - \frac{45\left|\hat{y}_2^b\right|^2\hat{\lambda}_{11,22}}{8} + \frac{45\left|\hat{y}_2^b\right|^2\hat{\lambda}_{12,21}}{8} + \frac{45\hat{\lambda}_{11,11}^2}{2} + \frac{15\hat{\lambda}_{11,22}^2}{4} + \frac{15\hat{\lambda}_{12,21}^2}{4}$$

$$+ \frac{15\hat{\lambda}_{11,22}\hat{\lambda}_{12,21}}{4} + \frac{45\hat{\lambda}_{12,12}\hat{\lambda}_{21,21}}{2} + \frac{135\hat{\lambda}_{11,12}\hat{\lambda}_{11,21}}{8} + \frac{45\hat{\lambda}_{12,22}\hat{\lambda}_{21,22}}{8}\Big)$$

$$+ \alpha_3\Big(-\frac{157\hat{y}^{t\,4}}{2} + \frac{27\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^2}{2} - \frac{185\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2}{12} + 41\left|\hat{y}_1^b\right|^4 + \frac{235\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2}{12}$$

$$- \frac{257\left|\hat{y}_2^b\right|^4}{12} + \zeta_3\Big(-16\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^2 - 12\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2 - 32\left|\hat{y}_1^b\right|^4 - 20\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2 + 12\left|\hat{y}_2^b\right|^4\Big)$$

$$+ 8\hat{y}^{t\,2}\hat{\lambda}_{11,11} + \frac{4\left|\hat{y}_2^b\right|^2\hat{\lambda}_{11,22}}{3} - \frac{4\left|\hat{y}_2^b\right|^2\hat{\lambda}_{12,21}}{3}\Big) + \frac{339\hat{y}^{t\,6}}{16} + \frac{739\hat{y}^{t\,4}\left|\hat{y}_1^b\right|^2}{32} + \frac{49\hat{y}^{t\,4}\left|\hat{y}_2^b\right|^2}{16}$$

$$+ \frac{825\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^4}{16} + \frac{671\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2}{16} + \frac{87\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^4}{8} + \frac{477\left|\hat{y}_1^b\right|^6}{32} + \frac{525\left|\hat{y}_1^b\right|^4\left|\hat{y}_2^b\right|^2}{16}$$

$$+ \frac{669\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^4}{32} + 3\left|\hat{y}_2^b\right|^6 + \zeta_3\Big(\frac{27\hat{y}^{t\,6}}{4} - 24\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^4 - 24\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2 + \frac{9\left|\hat{y}_1^b\right|^6}{4}$$

$$+ \frac{21\left|\hat{y}_1^b\right|^4\left|\hat{y}_2^b\right|^2}{4} + \frac{15\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^4}{4} + \frac{3\left|\hat{y}_2^b\right|^6}{4}\Big) + \hat{\lambda}_{11,11}\Big(99\hat{y}^{t\,4} + \frac{93\hat{y}^{t\,2}\left|\hat{y}_1^b\right|^2}{2}$$

$$+ \frac{3\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2}{2} + \frac{15\left|\hat{y}_1^b\right|^4}{2} + 6\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2\Big) + \hat{\lambda}_{11,22}\Big(\frac{23\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2}{2} + 11\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2$$

$$+ \frac{35\left|\hat{y}_2^b\right|^4}{4}\Big) + \hat{\lambda}_{12,21}\Big(-\frac{11\hat{y}^{t\,2}\left|\hat{y}_2^b\right|^2}{2} - \frac{7\left|\hat{y}_1^b\right|^2\left|\hat{y}_2^b\right|^2}{2} - \frac{23\left|\hat{y}_2^b\right|^4}{4}\Big)$$

$$+ \hat{\lambda}_{11,12}\Big(\frac{57\hat{y}^{t\,2}\hat{y}_1^b\hat{y}_2^{b\,*}}{4} + \frac{39\left|\hat{y}_1^b\right|^2\hat{y}_1^b\hat{y}_2^{b\,*}}{8} + 3\left|\hat{y}_2^b\right|^2\hat{y}_1^b\hat{y}_2^{b\,*}\Big) + \hat{\lambda}_{11,21}\Big(\frac{57\hat{y}^{t\,2}\hat{y}_1^{b\,*}\hat{y}_2^b}{4}$$

$$+ \frac{39\left|\hat{y}_1^b\right|^2\hat{y}_1^{b\,*}\hat{y}_2^b}{8} + 3\left|\hat{y}_2^b\right|^2\hat{y}_1^{b\,*}\hat{y}_2^b\Big) + 3\hat{\lambda}_{22,22}\left|\hat{y}_2^b\right|^4 + \frac{9\hat{\lambda}_{12,12}\left(\hat{y}_1^b\hat{y}_2^{b\,*}\right)^2}{4}$$

$$+ \frac{9\hat{\lambda}_{21,21}\left(\hat{y}_1^{b\,*}\hat{y}_2^b\right)^2}{4} + \frac{21\hat{\lambda}_{12,22}\left|\hat{y}_2^b\right|^2\hat{y}_1^b\hat{y}_2^{b\,*}}{8} + \frac{21\hat{\lambda}_{21,22}\left|\hat{y}_2^b\right|^2\hat{y}_1^{b\,*}\hat{y}_2^b}{8} + \hat{\lambda}_{11,11}^2\Big(\frac{15\hat{y}^{t\,2}}{8}$$

$$-\frac{291\left|\hat{y}_1^b\right|^2}{8}\Big) + \hat{\lambda}_{11,22}^2\Big(-\frac{15\hat{y}^{t2}}{16} - \frac{37\left|\hat{y}_1^b\right|^2}{16} - \frac{39\left|\hat{y}_2^b\right|^2}{16}\Big) + \hat{\lambda}_{12,21}^2\Big(-\frac{39\hat{y}^{t2}}{16}$$

$$+\frac{11\left|\hat{y}_1^b\right|^2}{16} - \frac{111\left|\hat{y}_2^b\right|^2}{16}\Big) - \frac{33\hat{\lambda}_{22,22}^2\left|\hat{y}_2^b\right|^2}{8} + \hat{\lambda}_{12,12}\hat{\lambda}_{21,21}\Big(-\frac{45\hat{y}^{t2}}{8} - \frac{15\left|\hat{y}_1^b\right|^2}{8}$$

$$-\frac{357\left|\hat{y}_2^b\right|^2}{8}\Big) + \hat{\lambda}_{11,12}\hat{\lambda}_{11,21}\Big(-\frac{69\hat{y}^{t2}}{32} - \frac{507\left|\hat{y}_1^b\right|^2}{32} - \frac{447\left|\hat{y}_2^b\right|^2}{32}\Big)$$

$$+\hat{\lambda}_{12,22}\hat{\lambda}_{21,22}\Big(-\frac{99\hat{y}^{t2}}{32} + \frac{75\left|\hat{y}_1^b\right|^2}{32} - \frac{513\left|\hat{y}_2^b\right|^2}{32}\Big) + \hat{\lambda}_{11,22}\hat{\lambda}_{12,21}\Big(-\frac{15\hat{y}^{t2}}{16}$$

$$-\frac{37\left|\hat{y}_1^b\right|^2}{16} - \frac{135\left|\hat{y}_2^b\right|^2}{16}\Big) + 3\hat{\lambda}_{11,11}\hat{\lambda}_{11,22}\left|\hat{y}_2^b\right|^2 + 3\hat{\lambda}_{11,22}\hat{\lambda}_{22,22}\left|\hat{y}_2^b\right|^2$$

$$-\frac{345\hat{\lambda}_{11,11}\hat{\lambda}_{11,12}\hat{y}_1^b\hat{y}_2^{b*}}{16} - \frac{345\hat{\lambda}_{11,11}\hat{\lambda}_{11,21}\hat{y}_1^{b*}\hat{y}_2^b}{16} - \frac{159\hat{\lambda}_{11,22}\hat{\lambda}_{11,12}\hat{y}_1^b\hat{y}_2^{b*}}{32}$$

$$-\frac{159\hat{\lambda}_{11,22}\hat{\lambda}_{11,21}\hat{y}_1^{b*}\hat{y}_2^b}{32} - \frac{165\hat{\lambda}_{11,22}\hat{\lambda}_{12,22}\hat{y}_1^b\hat{y}_2^{b*}}{32} - \frac{165\hat{\lambda}_{11,22}\hat{\lambda}_{21,22}\hat{y}_1^{b*}\hat{y}_2^b}{32}$$

$$-\frac{255\hat{\lambda}_{12,21}\hat{\lambda}_{11,12}\hat{y}_1^b\hat{y}_2^{b*}}{32} - \frac{255\hat{\lambda}_{12,21}\hat{\lambda}_{11,21}\hat{y}_1^{b*}\hat{y}_2^b}{32} - \frac{69\hat{\lambda}_{12,21}\hat{\lambda}_{12,22}\hat{y}_1^b\hat{y}_2^{b*}}{32}$$

$$-\frac{69\hat{\lambda}_{12,21}\hat{\lambda}_{21,22}\hat{y}_1^{b*}\hat{y}_2^b}{32} + \frac{21\hat{\lambda}_{22,22}\hat{\lambda}_{12,22}\hat{y}_1^b\hat{y}_2^{b*}}{16} + \frac{21\hat{\lambda}_{22,22}\hat{\lambda}_{21,22}\hat{y}_1^{b*}\hat{y}_2^b}{16}$$

$$-\frac{255\hat{\lambda}_{12,12}\hat{\lambda}_{11,21}\hat{y}_1^b\hat{y}_2^{b*}}{16} - \frac{255\hat{\lambda}_{21,21}\hat{\lambda}_{11,12}\hat{y}_1^{b*}\hat{y}_2^b}{16}$$

$$-\frac{69\hat{\lambda}_{12,12}\hat{\lambda}_{21,22}\hat{y}_1^b\hat{y}_2^{b*}}{16} - \frac{69\hat{\lambda}_{21,21}\hat{\lambda}_{12,22}\hat{y}_1^{b*}\hat{y}_2^b}{16} + \frac{3\hat{\lambda}_{11,12}\hat{\lambda}_{21,22}\left|\hat{y}_2^b\right|^2}{2}$$

$$+\frac{3\hat{\lambda}_{11,21}\hat{\lambda}_{12,22}\left|\hat{y}_2^b\right|^2}{2} - 18\hat{\lambda}_{11,11}^3 - \frac{\hat{\lambda}_{11,22}^3}{2} - \frac{5\hat{\lambda}_{12,21}^3}{8} - 3\hat{\lambda}_{11,11}\hat{\lambda}_{11,22}^2 - \frac{3\hat{\lambda}_{11,11}\hat{\lambda}_{12,21}^2}{2}$$

$$-3\hat{\lambda}_{11,11}\hat{\lambda}_{11,22}\hat{\lambda}_{12,21} - 6\hat{\lambda}_{11,11}\hat{\lambda}_{12,12}\hat{\lambda}_{21,21} - \frac{45\hat{\lambda}_{11,11}\hat{\lambda}_{11,12}\hat{\lambda}_{11,21}}{2} - \frac{3\hat{\lambda}_{11,22}^2\hat{\lambda}_{22,22}}{2}$$

$$-\frac{3\hat{\lambda}_{11,22}^2\hat{\lambda}_{12,21}}{4} - \frac{3\hat{\lambda}_{11,22}\hat{\lambda}_{12,21}\hat{\lambda}_{22,22}}{2} - \frac{3\hat{\lambda}_{11,22}\hat{\lambda}_{12,21}^2}{2} - \frac{9\hat{\lambda}_{11,22}\hat{\lambda}_{11,12}\hat{\lambda}_{11,21}}{2}$$

$$-\frac{27\hat{\lambda}_{11,22}\hat{\lambda}_{11,12}\hat{\lambda}_{21,22}}{8} - \frac{27\hat{\lambda}_{11,22}\hat{\lambda}_{11,21}\hat{\lambda}_{12,22}}{8} - 9\hat{\lambda}_{11,22}\hat{\lambda}_{12,12}\hat{\lambda}_{21,21} - \frac{9\hat{\lambda}_{11,22}\hat{\lambda}_{12,22}\hat{\lambda}_{21,22}}{4}$$

$$-\frac{3\hat{\lambda}_{12,21}^2\hat{\lambda}_{22,22}}{4} - 6\hat{\lambda}_{12,21}\hat{\lambda}_{11,21}\hat{\lambda}_{11,12} - \frac{9\hat{\lambda}_{12,21}\hat{\lambda}_{11,12}\hat{\lambda}_{21,22}}{4} - \frac{9\hat{\lambda}_{12,21}\hat{\lambda}_{11,21}\hat{\lambda}_{12,22}}{4}$$

$$-\frac{27\hat{\lambda}_{12,21}\hat{\lambda}_{12,12}\hat{\lambda}_{21,21}}{2} - 3\hat{\lambda}_{12,21}\hat{\lambda}_{12,22}\hat{\lambda}_{21,22} - 3\hat{\lambda}_{22,22}\hat{\lambda}_{12,12}\hat{\lambda}_{21,21} - \frac{15\hat{\lambda}_{11,12}^2\hat{\lambda}_{21,21}}{2}$$

$$-\frac{9\hat{\lambda}_{11,12}\hat{\lambda}_{21,21}\hat{\lambda}_{12,22}}{4} - \frac{15\hat{\lambda}_{11,21}^2\hat{\lambda}_{12,12}}{2} - \frac{9\hat{\lambda}_{11,21}\hat{\lambda}_{12,12}\hat{\lambda}_{21,22}}{4} - \frac{15\hat{\lambda}_{12,12}\hat{\lambda}_{21,22}^2}{4}$$

$$
\left. - \frac{15\hat{\lambda}_{21,21}\hat{\lambda}_{12,22}^2}{4} - \frac{9\hat{\lambda}_{22,22}\hat{\lambda}_{12,22}\hat{\lambda}_{21,22}}{2} \right], \tag{50}
$$

where also the quartic couplings are given in the new basis (cf. Eq. (8)). We rescaled all Yukawa couplings by $\hat{y} = y/\sqrt{4\pi}$ but the leading ones. The analytic expression of Eq. (50) and the beta functions for y_1^b and y_2^b are contained in ancillary files which come together with this paper [30]. They also contain the beta functions for the eleven invariants specified to the 2HDM models I, II, X and Y and the SM. We furthermore provide explicit results for the quantities in Eqs. (30) and (31).

Let us mention that for the SM Yukawa matrix beta functions we find full agreement with [4, 6] and the one- and two-loop beta functions for $\mathbb{Z}_2$-symmetric 2HDMs agree with [46].

7 Summary

We consider a general 2HDM and compute the beta functions for the gauge and Yukawa couplings up to three loops. We discuss in detail the subtleties in connection to the determination of the renormalization constants in case both Higgs doublets couple to up- and down-type fermions. Furthermore, we investigate in detail the origin of the poles in the Yukawa coupling beta functions, a characteristic which is already present in the SM, discuss their ambiguity, and provide possible solutions which lead to finite beta functions. Our general results can be specified to $\mathbb{Z}_2$ symmetric models like the 2HDMs of type I, II, X or Y, or the SM. In this paper we also provide the first independent cross check of the three-loop corrections to the SM Yukawa coupling beta functions [4,6]. Ancillary files with analytic results for both, renormalization constants and beta functions, can be downloaded from [30].

Acknowledgements

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