

Assessing boundedness from below in the $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetric three-Higgs-doublet model: Algorithm and machine learning

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Abstract

The scalar potential of any particle-physics model must be bounded from below (BFB). We consider the extension of the Standard electroweak Model with three $SU(2)$ doublets of scalars and a symmetry under which each of those doublets changes sign. In the absence of necessary and sufficient conditions for boundedness from below (BnessFB) for this specific model, we argue that one may use increasingly stringent sets of necessary conditions. We introduce a `Mathematica` code, `StableWein`, that implements this idea. The user is allowed to choose the level of accuracy that they want in the determination of BnessFB; more precision means the use of more necessary conditions, and usually entails a longer running time for the code. Our investigation suggests that our procedure and code can be extremely precise in the determination of the potentials that are BFB. In addition, we introduce a machine-learning code that identifies, with more than 99% accuracy, which potentials are BFB.



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1 Introduction

Throughout this paper, the renormalizable scalar potentials are of the form $V_2 + V_4$, where V_2 is quadratic in the scalar fields and V_4 is quartic in the scalar fields.

In the extremely successful Standard Model (SM) of the electroweak interactions, the gauge group is $SU(2) \times U(1)$ and there is only one $SU(2)$ doublet of scalars: Φ . Hence, $V_2 = \mu \Phi^\dagger \Phi$ and $V_4 = \lambda (\Phi^\dagger \Phi)^2$, where μ and λ are couplings, *i.e.* numbers (not fields).

The consistency of any particle-physics model necessitates that its scalar potential is bounded from below (BFB). This means that the potential can never tend to minus infinity—else the Hamiltonian does not have a minimum, *i.e.* the theory has no vacuum state. Boundedness from below (BnessFB) is equivalent to V_4 being positive for any values of the scalar fields.¹ If V_4 were negative for some values of the scalar fields, then multiplying those values by an ever-increasing positive number would make the potential tend to minus infinity. In the SM, since $\Phi^\dagger \Phi \geq 0$, the potential is BFB if and only if λ is positive.

For a variety of reasons—like accommodating nonzero neutrino masses, dark matter, and baryogenesis²—many particle physicists like to extend the SM. Most extensions have a scalar sector larger than the one of the SM, in particular more than one $SU(2)$ doublet. (There are also extensions of the SM with a larger gauge group.) The scalar sector of the two-Higgs-doublet model (2HDM) [2] has been extensively explored. This paper concentrates on the model with three scalar $SU(2)$ doublets Φ_k ($k = 1, 2, 3$ throughout this paper), which is called the three-Higgs-doublet model (3HDM).³

Unfortunately, for all but the simplest extensions of the SM V_4 has many couplings—not just one, like λ in the SM—and it is not possible to establish mathematical necessary and sufficient conditions for BnessFB in terms of those couplings alone. This has been achieved [3] for the 2HDM, where V_4 has $2^2(2^2 + 1)/2 = 10$ real couplings; for the 3HDM, where V_4 has $3^2(3^2 + 1)/2 = 45$ real couplings [4], it could not be achieved.

However, most 3HDMs used in practical models have additional (non-gauge, or ‘internal’) symmetries. Those symmetries restrict V_4 , making it have much less than 45 real couplings. The symmetries that the scalar potential of a 3HDM may enjoy have been classified. Some of

¹When one uses our condition that V_4 be *positive* for any values of the scalar fields, V_2 is irrelevant for BnessFB. The weaker condition where V_4 is allowed to be zero necessitates that one furthermore makes sure that $V_2 \geq 0$ whenever $V_4 = 0$. This may be tricky [1], therefore we prefer the stricter condition $V_4 > 0$.

²In the SM there is neither sufficient CP violation nor the first-order phase transition necessary for baryogenesis.

³There are many 3HDMs, depending both on the additional symmetries that are imposed and on the fermionic sector.

them have a $U(1)_1 \times U(1)_2$ subgroup, where

$$U(1)_1 : \quad \Phi_2 \rightarrow e^{i\varrho} \Phi_2, \quad \Phi_3 \rightarrow e^{-i\varrho} \Phi_3, \quad (1a)$$

$$U(1)_2 : \quad \Phi_1 \rightarrow e^{2i\varsigma} \Phi_1, \quad \Phi_2 \rightarrow e^{-i\varsigma} \Phi_2, \quad \Phi_3 \rightarrow e^{-i\varsigma} \Phi_3. \quad (1b)$$

In Eqs. (1), ϱ and ς are arbitrary phases. Other internal symmetries have just a $\mathbb{Z}_2^{(3)} \times U(1)_2$ subgroup, where $\mathbb{Z}_2^{(3)}$ is generated by the transformation

$$\mathbb{Z}_2^{(3)} : \quad \Phi_3 \rightarrow -\Phi_3. \quad (2)$$

Still other internal symmetries have only a $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ subgroup,⁴ where $\mathbb{Z}_2^{(2)}$ is generated by the transformation

$$\mathbb{Z}_2^{(2)} : \quad \Phi_2 \rightarrow -\Phi_2. \quad (3)$$

Finally, there are internal symmetries that do not have any of these subgroups. All possible internal symmetries of the renormalizable potential of a 3HDM are listed in Appendix A.

So, usually one does not need to establish whether the potential of the full 3HDM is BFB—one only has to do it for a V_4 constrained by a symmetry, hence with less than 45 real couplings. Notably, a mathematical algorithm for deciding on the BnessFB of a potential with $U(1)_1 \times U(1)_2$ symmetry has been devised [8] and extended to a potential with $\mathbb{Z}_2^{(3)} \times U(1)_2$ symmetry [9]. The problem of the BnessFB of a potential with only $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ symmetry remains extant.⁵

Sufficient conditions for BnessFB of a $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric 3HDM potential have been devised [12, 13]. They have the obvious setback that one will be exploring only the portion of the space of BFB potentials that fulfill the sufficient conditions, neglecting other, potentially physically interesting parts of that space. In this paper, we contend that, in the case of $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric potentials, it is possible to take the alternative approach of using *necessary*, instead of sufficient, BnessFB conditions. In our approach, one incurs the risk of using potentials that fulfill the necessary conditions but are not really BFB; however, that risk may be systematically curtailed by using more and more necessary conditions, as we shall illustrate in this paper, thus diminishing the number of non-BFB potentials that one admits for analysis. Our explorations suggest that it is possible, without excessive computational effort, to utilize a set of necessary conditions that decides, *with extremely high accuracy* (much above 99%), which $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric 3HDM potentials are BFB.

This paper introduces the Mathematica package *StableWein* that encodes the result of our findings. The user of that notebook inputs the quartic part of a $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric potential and receives as output the indication of whether that potential is (likely to be) BFB or not. The level of precision of that indication may be chosen by the user: a greater level of precision means that more necessary conditions are employed and, consequently, the code takes a longer time to reach the indication. One further option of our code minimizes V_4 through brute force, in principle obtaining—if the minimization has been well done—the exact answer to the BnessFB question for that potential. Our code may be employed either for CP -violating $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric potentials or for CP -conserving ones; in the two cases the

⁴The 3HDM firstly (to our knowledge) used in particle physics had $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ symmetry [5, 6]. Inspired by Ref. [5], we call ‘Weinberg model’ to a 3HDM with $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ symmetry. This, together with some authors’ use of designating the conditions for BnessFB as ‘vacuum stability conditions’, is the origin of the name *StableWein* of the package introduced in this paper. The $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric 3HDM furnished with (spontaneously broken) CP symmetry was pioneered in Ref. [7]; we call it ‘Branco model’.

⁵The exception are the potentials with either S_4 or $SO(3)$ symmetries [10, 11] (see the third column of Table 5). However, those symmetries are much stronger than just $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$.

code uses somewhat different necessary conditions, and it achieves greater precision in the CP -conserving case (which has one parameter less in V_4).

Additionally, this paper also introduces neural networks (NNs)⁶ that have been trained to identify BFB $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric potentials; they too are implemented in the `StableWein` package. This artificial intelligence, which uses neither sufficient nor necessary BFB conditions, displays an accuracy close to 99.9% in deciding which potentials are BFB.

This paper is organized as follows. In Sec. 2 we derive necessary conditions for BnessFB of a $\mathbb{Z}_2 \times \mathbb{Z}_2$ -invariant 3HDM potential. In Sec. 3 we particularize the conditions of Sec. 2 to a CP -conserving potential. In Sec. 4 we provide sufficient conditions for BnessFB. In Sec. 5 we describe the minimization procedures used. In Sec. 6 we give instructions for using the package `StableWein`. The main conclusions of this paper are summarized in Sec. 7. Two appendices, which may be altogether omitted, deal on known material: Appendix A lists the possible symmetries of a 3HDM; Appendix B reviews the perturbative unitarity constraints for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ -invariant V_4 .

2 The necessary conditions for BnessFB

We refer to the $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetric 3HDM as Weinberg model. In this section, we define the three $SU(2)$ scalar doublets together with the quartic part of the scalar potential V_4 . We introduce the phase space coordinates ϖ_k and ϑ_k and present the copositivity condition on V_4 , from which we derive several sets of necessary conditions with increasing levels of accuracy. Throughout, we use $k = 1, 2, 3$.

Doublets: We write

$$\Phi_1 = \begin{pmatrix} a \\ b \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} c \\ d \end{pmatrix}, \quad \Phi_3 = \begin{pmatrix} e \\ f \end{pmatrix}, \quad (4)$$

where $a, \dots, f$ are complex scalar (Klein–Gordon) fields. Under an $SU(2) \times U(1)$ transformation $\Phi_k \rightarrow U_2 \Phi_k \forall k$, where U_2 is a matrix of $U(2)$.⁷ Without loss of generality, it is possible to make $a = 0$ everywhere in space–time through a (local) $SU(2)$ transformation, and then to make both b and c real through two (local) $U(1)$ transformations—one of them being the $U(1)$ in $SU(2) \times U(1)$ and the other one being the neutral component of $SU(2)$.

Parameters ϖ_k and ϑ_k : Assuming $\Phi_k^\dagger \Phi_k \neq 0 \forall k$,⁸ we define

$$\pi_1 := \frac{(\Phi_2^\dagger \Phi_3)^2}{\Phi_2^\dagger \Phi_2 \Phi_3^\dagger \Phi_3}, \quad \pi_2 := \frac{(\Phi_3^\dagger \Phi_1)^2}{\Phi_3^\dagger \Phi_3 \Phi_1^\dagger \Phi_1}, \quad \pi_3 := \frac{(\Phi_1^\dagger \Phi_2)^2}{\Phi_1^\dagger \Phi_1 \Phi_2^\dagger \Phi_2}. \quad (5)$$

We moreover define

$$\varpi_k := |\pi_k|, \quad \vartheta_k := \arg \pi_k, \quad \vartheta := \sum_{k=1}^3 \vartheta_k. \quad (6)$$

⁶See Ref. [14] for a paper where an NN is used to analyze a 3HDM, albeit one with $\mathbb{Z}_3$ instead of $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry and with emphasis elsewhere rather than on the BFB constraints on V_4 .

⁷Note that $U(2) \cong [SU(2) \times U(1)]/\mathbb{Z}_2$ is locally identical to $SU(2) \times U(1)$, but the two groups have different topologies. See for instance Ref. [15].

⁸If $\exists k : \Phi_k^\dagger \Phi_k = 0$, then the 3HDM reduces to a 2HDM, and the BFB conditions for a 2HDM are known. See below.

The ϖ_k satisfy

$$0 \leq \varpi_k \leq 1. \quad (7)$$

The six dimensionless parameters ϖ_k and ϑ_k are not independent, because

$$2(1 + \cos \vartheta) \prod_{k=1}^3 \varpi_k = \left(1 - \sum_{k=1}^3 \varpi_k\right)^2. \quad (8)$$

Equation (8) has been derived in Ref. [10] and follows from substituting Eqs. (4) in Eqs. (5).⁹ It implies that $\cos \vartheta \geq 0$ and leaves the sign of ϑ un-determined. Because of Eq. (8),

$$4 \prod_{k=1}^3 \varpi_k \geq \left(1 - \sum_{k=1}^3 \varpi_k\right)^2, \quad (9)$$

which constrains only the ϖ_k .

Special points: Using the notation $(\varpi_1, \varpi_2, \varpi_3)$, the four points

$$P_1 = (1, 0, 0), \quad P_2 = (0, 1, 0), \quad P_3 = (0, 0, 1), \quad P_4 = (1, 1, 1), \quad (10)$$

saturate the inequality (9). They are the corners of the allowed volume in $(\varpi_1, \varpi_2, \varpi_3)$ space, which is displayed in Fig. 1. Point P_1 is reached, for instance, when $a = d = f = 0$; point P_4 is reached when $a = c = e = 0$ (i.e. when all three doublets only have ‘neutral’ components [8] or are equivalent to singlets). Using Eq. (8) one sees that $\vartheta = 0$ at point P_4 , while points P_k have un-determined ϑ . As a matter of fact, ϑ is un-determined at the three edges connecting P_1, P_2 , and P_3 , and ϑ is zero at the whole rest of the surface that bounds the allowed $(\varpi_1, \varpi_2, \varpi_3)$ volume. At the center of the allowed volume, given by $\varpi_k = 1/2 \forall k$, $\cos \vartheta = 0$.

Potential: The $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric 3HDM has quartic potential

$$V_4 = \sum_{k=1}^3 \frac{a_k}{2} (\Phi_k^\dagger \Phi_k)^2 \quad (11a)$$

$$+ b_1 \Phi_2^\dagger \Phi_2 \Phi_3^\dagger \Phi_3 + b_2 \Phi_3^\dagger \Phi_3 \Phi_1^\dagger \Phi_1 + b_3 \Phi_1^\dagger \Phi_1 \Phi_2^\dagger \Phi_2 \quad (11b)$$

$$+ c_1 \Phi_2^\dagger \Phi_3 \Phi_3^\dagger \Phi_2 + c_2 \Phi_3^\dagger \Phi_1 \Phi_1^\dagger \Phi_3 + c_3 \Phi_1^\dagger \Phi_2 \Phi_2^\dagger \Phi_1 \quad (11c)$$

$$+ \left[e^{i\epsilon_1} \frac{d_1}{2} (\Phi_2^\dagger \Phi_3)^2 + e^{i\epsilon_2} \frac{d_2}{2} (\Phi_3^\dagger \Phi_1)^2 + e^{i\epsilon_3} \frac{d_3}{2} (\Phi_1^\dagger \Phi_2)^2 + \text{H.c.} \right], \quad (11d)$$

with twelve real couplings a_k, b_k, c_k , and d_k . The three phases ϵ_k are not all physical; only

$$\epsilon := \sum_{k=1}^3 \epsilon_k \quad (12)$$

has physical significance. Indeed, by changing the relative phases of the three doublets via $U(1)$ transformations, one may change the three ϵ_k , but ϵ remains invariant. In particular, one may re-write line (11d) in any one of the following three forms:

$$+ \left[e^{i\epsilon} \frac{d_1}{2} (\Phi_2^\dagger \Phi_3)^2 + \frac{d_2}{2} (\Phi_3^\dagger \Phi_1)^2 + \frac{d_3}{2} (\Phi_1^\dagger \Phi_2)^2 + \text{H.c.} \right], \quad (13a)$$

$$+ \left[\frac{d_1}{2} (\Phi_2^\dagger \Phi_3)^2 + e^{i\epsilon} \frac{d_2}{2} (\Phi_3^\dagger \Phi_1)^2 + \frac{d_3}{2} (\Phi_1^\dagger \Phi_2)^2 + \text{H.c.} \right], \quad (13b)$$

$$+ \left[\frac{d_1}{2} (\Phi_2^\dagger \Phi_3)^2 + \frac{d_2}{2} (\Phi_3^\dagger \Phi_1)^2 + e^{i\epsilon} \frac{d_3}{2} (\Phi_1^\dagger \Phi_2)^2 + \text{H.c.} \right]. \quad (13c)$$

⁹Equation (8) would not apply if the Φ_k were triplets of $SU(3)$ instead of doublets of $SU(2)$. On the other hand, if the Φ_k were singlets instead of doublets, then the much stronger equations $\vartheta = 0$ and $\varpi_k = 1 \forall k$ would hold.

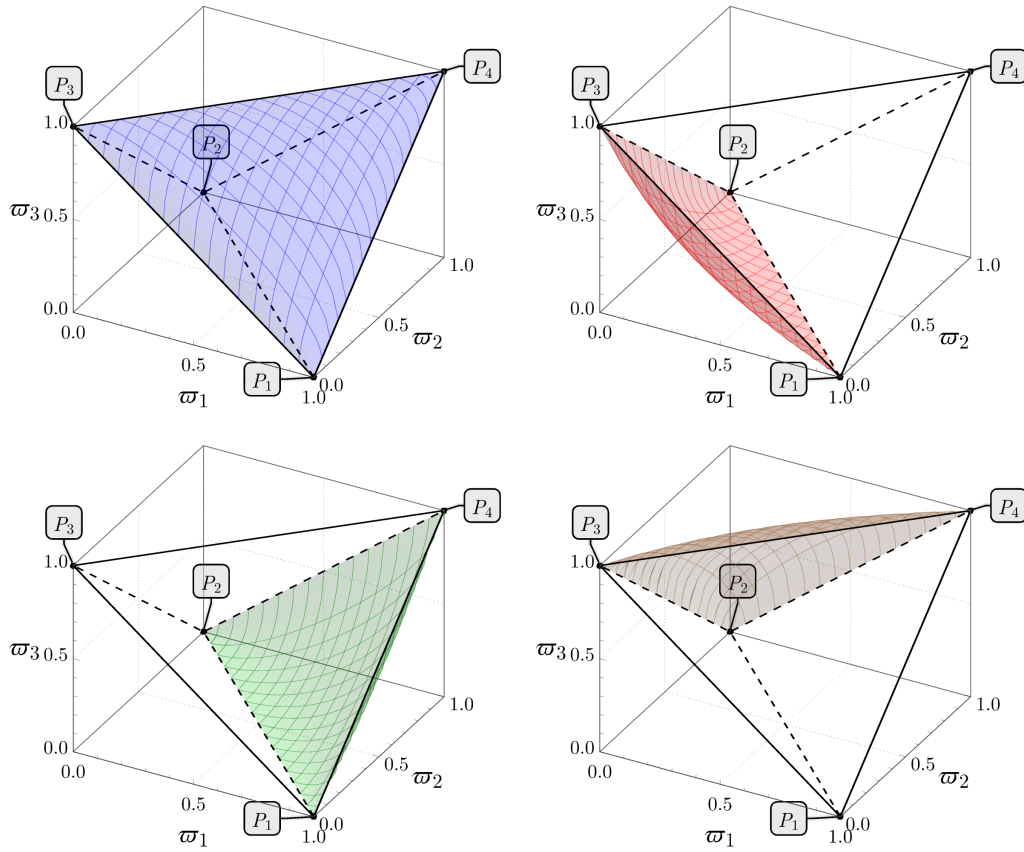


Figure 1: A perspective of the allowed volume in $(\varpi_1, \varpi_2, \varpi_3)$ space. The four points $P_{1,2,3,4}$ defined in Eqs. (10) are displayed. The three edges connecting P_1 , P_3 , and P_4 are displayed as full straight lines; the edges connecting each of those three points to P_2 are dashed lines. In each of the four panels of the figure, the four faces of the surface that bounds the allowed volume are separately displayed in different colours; in each case, a darker tone colours the part of the face that is visible in this perspective, and a lighter tone marks the part of the face that is hidden behind the volume. The four faces are identical and convex.

Thus, V_4 has 13 real couplings—the a_k , b_k , c_k , d_k , and ϵ —as advertised in the previous section. The perturbative unitarity bounds on those 13 parameters are given in Appendix B; they have been implemented in `StableWein`.

NCL1: Using the definitions (5) and (6), one may re-write Eq. (11) as

$$V_4 = \frac{1}{2} \begin{pmatrix} \Phi_1^\dagger \Phi_1 & \Phi_2^\dagger \Phi_2 & \Phi_3^\dagger \Phi_3 \end{pmatrix} M \begin{pmatrix} \Phi_1^\dagger \Phi_1 \\ \Phi_2^\dagger \Phi_2 \\ \Phi_3^\dagger \Phi_3 \end{pmatrix}, \quad (14)$$

where M is a real and symmetric matrix:

$$M = \begin{pmatrix} a_1 & b_3 + X_3 & b_2 + X_2 \\ b_3 + X_3 & a_2 & b_1 + X_1 \\ b_2 + X_2 & b_1 + X_1 & a_3 \end{pmatrix}. \quad (15)$$

In Eq. (15),

$$X_k := c_k \varpi_k + d_k \operatorname{Re}(e^{i\epsilon_k} \pi_k) = \varpi_k [c_k + d_k \cos(\epsilon_k + \vartheta_k)]. \quad (16)$$

BnessFB means that V_4 is **positive** for any values of the fields $a, \dots, f$. Since in Eq. (14) $\Phi_k^\dagger \Phi_k > 0 \forall k$, this is equivalent to the matrix M being **strictly** copositive [16]. The conditions for **strict** copositiveness are¹⁰

$$a_1 > 0, \quad (17a)$$

$$a_2 > 0, \quad (17b)$$

$$a_3 > 0, \quad (17c)$$

$$B_1 \equiv b_1 + \sqrt{a_2 a_3} + X_1 > 0, \quad (17d)$$

$$B_2 \equiv b_2 + \sqrt{a_3 a_1} + X_2 > 0, \quad (17e)$$

$$B_3 \equiv b_3 + \sqrt{a_1 a_2} + X_3 > 0, \quad (17f)$$

$$P + Q > 0, \quad (17g)$$

where

$$P \equiv \sqrt{\prod_{k=1}^3 a_k} + \sum_{k=1}^3 (b_k + X_k) \sqrt{a_k}, \quad (18a)$$

$$Q \equiv \sqrt{2B_1 B_2 B_3}. \quad (18b)$$

BnessFB is equivalent to Eqs. (17) holding for all possible values of the π_k . Using Eq. (16), conditions (17d)–(17f) may be written as

$$\varpi_k [c_k + d_k \cos(\varepsilon_k + \vartheta_k)] > -\bar{b}_k, \quad (19)$$

where

$$\bar{b}_1 := b_1 + \sqrt{a_2 a_3}, \quad \bar{b}_2 := b_2 + \sqrt{a_3 a_1}, \quad \bar{b}_3 := b_3 + \sqrt{a_1 a_2}. \quad (20)$$

Since each ϖ_k may take any value between 0 and 1, and since each ϑ_k may take any value between 0 and 2π , condition (19) is equivalent to $0 > -\bar{b}_k$ and $c_k - |d_k| > -\bar{b}_k$. So, altogether conditions (17a)–(17f) are equivalent to the “necessary conditions of level 1” (NCL1), viz.

$$\text{NCL1:} \quad a_k > 0, \quad \bar{b}_k > 0, \quad \bar{b}_k + e_k > 0, \quad \forall k = 1, 2, 3, \quad (21)$$

where

$$e_k := c_k - |d_k|. \quad (22)$$

Only condition (17g), viz.

$$\sum_{k=1}^3 X_k \sqrt{a_k} + \sqrt{2 \prod_{k=1}^3 (\bar{b}_k + X_k)} > -\bar{a}, \quad (23)$$

remains to be taken care of. In inequality (23),

$$\bar{a} := \sqrt{\prod_{k=1}^3 a_k} + \sum_{k=1}^3 b_k \sqrt{a_k}. \quad (24)$$

The NCL1, *i.e.* conditions (21), are necessary conditions for BnessFB. They are well known: for instance the fields e and f are zero, *i.e.* if the doublet Φ_3 is zero, then one has the 2HDM formed by only Φ_1 and Φ_2 and with symmetry $\mathbb{Z}_2^{(2)}$; the conditions $a_1 > 0$, $a_2 > 0$, $\bar{b}_3 > 0$, and $\bar{b}_3 + e_3 > 0$ are precisely the BFB conditions for that 2HDM [2]. Thus, the NCL1 may be obtained by considering the three 2HDMs that are sub-cases of the 3HDM.

¹⁰Since $Q > 0$, condition (17g) is equivalent to either $P \geq 0$ or $P^2 < Q^2$; the latter condition is equivalent to $\det M > 0$.

NCL2: In order to go beyond conditions (21) one must use inequality (23). One possibility is enforcing that inequality at the points P_k . Using Eq. (16) one sees that, for instance at point P_1 where $\varpi_2 = \varpi_3 = 0$ and $\varpi_1 = 1$, $X_2 = X_3 = 0$ and the minimum possible value of X_1 is e_1 . One thus obtains for P_1 , P_2 , and P_3 ,

$$\text{NCL2 : } \begin{cases} e_1 \sqrt{a_1} + \sqrt{2(\bar{b}_1 + e_1) \bar{b}_2 \bar{b}_3} > -\bar{a}, \\ e_2 \sqrt{a_2} + \sqrt{2\bar{b}_1 (\bar{b}_2 + e_2) \bar{b}_3} > -\bar{a}, \\ e_3 \sqrt{a_3} + \sqrt{2\bar{b}_1 \bar{b}_2 (\bar{b}_3 + e_3)} > -\bar{a}, \end{cases} \quad (25)$$

respectively. Inequalities (25) are necessary conditions for BnessFB; we call them the “necessary conditions of level 2 (NCL2).”

NCL3: Let us fix $\vartheta = 0$. Condition (23) then reads

$$\begin{aligned} & \varpi_1 [c_1 + d_1 \cos(\varepsilon - \vartheta_2 - \vartheta_3)] \sqrt{a_1} + \sum_{j=2}^3 \varpi_j (c_j + d_j \cos \vartheta_j) \sqrt{a_j} \\ & + \sqrt{2 \{ \bar{b}_1 + \varpi_1 [c_1 + d_1 \cos(\varepsilon - \vartheta_2 - \vartheta_3)] \} \prod_{j=2}^3 [\bar{b}_j + \varpi_j (c_j + d_j \cos \vartheta_j)]} > -\bar{a}, \end{aligned} \quad (26)$$

where we have opted for the choice $\varepsilon_1 = \varepsilon$ and $\varepsilon_2 = \varepsilon_3 = 0$. Inequality (26) must hold for all $\vartheta_2, \vartheta_3 \in [0, 2\pi[$ and for all ϖ_k that satisfy Eq. (8) with $\vartheta = 0$, viz. with

$$\varpi_1 = \left[\sqrt{\varpi_2 \varpi_3} \pm \sqrt{(1 - \varpi_2)(1 - \varpi_3)} \right]^2. \quad (27)$$

So, there are four degrees of freedom ϑ_2 , ϑ_3 , ϖ_2 , and ϖ_3 in inequality (26). One may reduce them to two degrees of freedom in, for instance, one of the following two ways:

1. One may consider point P_4 which, besides having $\vartheta = 0$, also has $\varpi_1 = \varpi_2 = \varpi_3 = 1$. Inequality (26) then reads

$$\begin{aligned} & [c_1 + d_1 \cos(\varepsilon - \vartheta_2 - \vartheta_3)] \sqrt{a_1} + \sum_{j=2}^3 (c_j + d_j \cos \vartheta_j) \sqrt{a_j} \\ & + \sqrt{2 [\bar{b}_1 + c_1 + d_1 \cos(\varepsilon - \vartheta_2 - \vartheta_3)] \prod_{j=2}^3 (\bar{b}_j + c_j + d_j \cos \vartheta_j)} > -\bar{a}. \end{aligned} \quad (28)$$

Inequality (28) must hold for all values of the phases ϑ_2 and ϑ_3 . In particular, one may choose both ϑ_2 and ϑ_3 to take one of the four values $\{0, \pi/2, \pi, 3\pi/2\}$; one then obtains

$$\text{NCL3 : } \sum_{k=1}^3 \beth_k \sqrt{a_k} + \sqrt{2 \prod_{k=1}^3 (\bar{b}_k + \beth_k)} > -\bar{a}, \quad (29)$$

with each of the following seven options for the $\beth_k$:

$$\beth_1 = c_1 + d_1 \cos \varepsilon, \quad \beth_2 = c_2 + d_2, \quad \beth_3 = c_3 + d_3, \quad (30a)$$

$$\beth_1 = c_1 + d_1 \cos \varepsilon, \quad \beth_2 = c_2 - d_2, \quad \beth_3 = c_3 - d_3, \quad (30b)$$

$$\beth_1 = c_1 - d_1 \cos \varepsilon, \quad \beth_2 = c_2 - d_2, \quad \beth_3 = c_3 + d_3, \quad (30c)$$

$$\beth_1 = c_1 - d_1 \cos \varepsilon, \quad \beth_2 = c_2 + d_2, \quad \beth_3 = c_3 - d_3, \quad (30d)$$

$$\beth_1 = c_1 - |d_1 \cos \varepsilon|, \quad \beth_2 = c_2, \quad \beth_3 = c_3, \quad (30e)$$

$$\beth_1 = c_1 - |d_1 \sin \varepsilon|, \quad \beth_2 = c_2, \quad \beth_3 = e_3. \quad (30f)$$

$$\beth_1 = c_1 - |d_1 \sin \varepsilon|, \quad \beth_2 = e_2, \quad \beth_3 = c_3. \quad (30g)$$

Since we might instead have opted for either of the choices $\varepsilon_2 = \varepsilon$ and $\varepsilon_1 = \varepsilon_3 = 0$, or $\varepsilon_3 = \varepsilon$ and $\varepsilon_1 = \varepsilon_2 = 0$, one must also consider all the possibilities (30) after permutation of the indices 1, 2, and 3. Our “necessary conditions of level 3 (NCL3)” for BnessFB are inequality (29) with each of the seven choices (30), together with their counterparts after permutation of the indices 1, 2, and 3, making a total of 21 inequalities.

2. One may choose both ϑ_2 and ϑ_3 to take one of the four values $\{0, \pi/2, \pi, 3\pi/2\}$ while keeping both ϖ_2 and ϖ_3 free. Inequality (26) then reads

$$\left[\sqrt{\varpi_2 \varpi_3} \pm \sqrt{(1-\varpi_2)(1-\varpi_3)} \right]^2 \beth_1 \sqrt{a_1} + \sum_{j=2}^3 \varpi_j \beth_j \sqrt{a_j} + \sqrt{2 \left\{ \bar{b}_1 + \left[\sqrt{\varpi_2 \varpi_3} \pm \sqrt{(1-\varpi_2)(1-\varpi_3)} \right]^2 \beth_1 \right\} \prod_{j=2}^3 (\bar{b}_j + \varpi_j \beth_j)} > -\bar{a}, \quad (31)$$

with each of the seven choices for the $\beth_k$ displayed in Eqs. (30).

NCL4: One may choose the alternative route of using inequality (28) keeping ϑ_2 and ϑ_3 free, together with inequality (31) with free ϖ_2 and ϖ_3 . Our “necessary conditions of level 4 (NCL4)” for BnessFB consist of scanning inequality (28) over both $\vartheta_2 \in [0, 2\pi[$ and $\vartheta_3 \in [0, 2\pi[$, together with scanning inequality (31)—with both signs “+” and “−”, and with all the 21 possibilities for the $\beth_k$ in Eqs. (30) and their counterparts with interchanged indices 1, 2, and 3—over both $\varpi_2 \in]0, 1]$ and $\varpi_3 \in]0, 1]$. In order to achieve greater accuracy, one may additionally scan the inequality (26) by fixing $\vartheta_2 = \pi$ and varying $\vartheta_3 \in [0, 2\pi[$ (and, conversely, fixing $\vartheta_3 = \pi$ and varying $\vartheta_2 \in [0, 2\pi[$), while simultaneously scanning $\varpi_{2,3} \in]0, 1]$. The same procedure may be repeated for the corresponding configurations obtained by permuting the indices 1, 2, and 3.

It should be emphasized that the inequalities in NCL2–NCL4 were selected on the basis of a painstaking study of the minimization of the left-hand side of Eq. (23). Namely, the left-hand side of Eq. (23) tends to attain minimal values for certain regions of the parameter space spanned by the ϖ_k and ϑ_k . The inequalities in NCL2–NCL4 are the ones with strongest discriminating power for testing BnessFB.

3 CP-conserving case

We refer to the CP-conserving $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric V_4 as Branco model. In that V_4 , the phases ε_k satisfy $\varepsilon = 0$. Consequently, the necessary BFB conditions NCL1–NCL4 of section 2 apply with $\varepsilon = 0$. In particular, the NCL1 and NCL2 do not depend on the ε_k . The NCL3 are given by Eq. (29), with $\beth_k$ chosen according to each of the following seven options:

$$\beth_1 = c_1 + d_1, \quad \beth_2 = c_2 + d_2, \quad \beth_3 = c_3 + d_3, \quad (32a)$$

$$\beth_1 = c_1 + d_1, \quad \beth_2 = c_2 - d_2, \quad \beth_3 = c_3 - d_3, \quad (32b)$$

$$\beth_1 = c_1 - d_1, \quad \beth_2 = c_2 - d_2, \quad \beth_3 = c_3 + d_3, \quad (32c)$$

$$\beth_1 = c_1 - d_1, \quad \beth_2 = c_2 + d_2, \quad \beth_3 = c_3 - d_3, \quad (32d)$$

$$\beth_1 = e_1, \quad \beth_2 = c_2, \quad \beth_3 = c_3, \quad (32e)$$

$$\beth_1 = c_1, \quad \beth_2 = e_2, \quad \beth_3 = c_3, \quad (32f)$$

$$\beth_1 = c_1, \quad \beth_2 = c_2, \quad \beth_3 = e_3. \quad (32g)$$

The NCL4 are implemented by scanning inequality

$$[c_1 + d_1 \cos(\vartheta_2 + \vartheta_3)] \sqrt{a_1} + \sum_{j=2}^3 (c_j + d_j \cos \vartheta_j) \sqrt{a_j} + \sqrt{2[\bar{b}_1 + c_1 + d_1 \cos(\vartheta_2 + \vartheta_3)] \prod_{j=2}^3 (\bar{b}_j + c_j + d_j \cos \vartheta_j)} > -\bar{a}, \quad (33)$$

over both $\vartheta_2 \in [0, 2\pi[$ and $\vartheta_3 \in [0, 2\pi[$, in combination with scanning inequality (31) over $\varpi_2 \in]0, 1]$ and $\varpi_3 \in]0, 1]$, for each sign choice and with the $\mathfrak{I}_k$ defined in each of Eqs. (32).

4 Sufficient conditions

According to Ref. [12], sufficient conditions for BnessFB of the quartic potential (11) are

$$a_k > 0, \quad (34a)$$

$$f_1 > -\sqrt{a_2 a_3}, \quad (34b)$$

$$f_2 > -\sqrt{a_3 a_1}, \quad (34c)$$

$$f_3 > -\sqrt{a_1 a_2}, \quad (34d)$$

and either

$$\sum_{k=1}^3 f_k \sqrt{a_k} > 0 \quad (35)$$

or

$$\prod_{k=1}^3 a_k + 2 \prod_{k=1}^3 f_k - \sum_{k=1}^3 a_k f_k^2 > 0, \quad (36)$$

where

$$f_k := b_k + \min(0, e_k). \quad (37)$$

According to Ref. [13], sufficient conditions for BnessFB of the quartic potential (11) are

$$a_k > 0, \quad (38a)$$

$$\bar{g}_k > 0, \quad (38b)$$

$$\sqrt{\prod_{k=1}^3 a_k} + \sum_{k=1}^3 g_k \sqrt{a_k} + \sqrt{2 \prod_{k=1}^3 \bar{g}_k} > 0. \quad (38c)$$

Here,

$$g_k := b_k + \min(0, c_k) - |d_k|, \quad (39)$$

and

$$\bar{g}_1 := g_1 + \sqrt{a_2 a_3}, \quad \bar{g}_2 := g_2 + \sqrt{a_3 a_1}, \quad \bar{g}_3 := g_3 + \sqrt{a_1 a_2}. \quad (40)$$

Note that none of these two sets of sufficient conditions involves the parameters ε ; they coincide for Weinberg model and Branco model.

We have numerically confirmed that each of these two sets of sufficient conditions selects a subset of the true BFB region but excludes regions that are also BFB. Moreover, neither of the two subsets selected by conditions (34)–(36) and (38) is a subset of the other subset. Last but not least, we have found that the conditions (38) exclude a substantially larger portion of parameter space than conditions (34)–(36).

5 Minimization of the potential

Our analysis required the global minimization of V_4 for several purposes:

- In order to confirm that the quartic potentials that satisfy the sufficient conditions for BnessFB [12, 13] really are BFB.
- In order to confirm that all the BFB quartic potentials do satisfy the necessary conditions for BnessFB.
- In order to quantify the accuracy of the necessary conditions, *i.e.* to find out the percentage of the potentials that obey those conditions which are *not* BFB.
- In order to prepare training data for our NNs.

For the minimization we have used the `Mathematica` function `NMinimize`. Since that function operates on real variables, the complex scalar fields were decomposed into their real and imaginary components. We fixed $a = 0$ and $b = 1$ and we minimized V_4 relative to the remaining fields. Fixing $a = 0$ is always possible via a local $SU(2) \times U(1)$ transformation and allows one to reduce the number of real variables by two. Fixing $b = 1$ further reduces the number of real variables by one and improves the stability of the numerical minimization, without entailing any lack of generality, since it simply corresponds to a re-scaling of all the nonzero fields b, c, d, e , and f . Note that the particular case $a = b = 0$ requires no separate treatment as it corresponds to the 2HDM formed by the doublets Φ_2 and Φ_3 , for which the necessary and sufficient BnessFB conditions are NCL1.

Global minimization is computationally very demanding and may return a local minimum instead of the global one. In order to improve robustness and accuracy, we employed the following strategies:

- Minimization with multiple algorithms, including Nelder–Mead and Differential Evolution.¹¹
- Minimization both with the default numerical precision and with increased precision.
- Minimization over multiple field ranges, *i.e.* allowing the real and imaginary parts of c, d, e , and f to vary from $-m$ to $+m$ for various values of the positive number m .
- In Weinberg model, minimization of V_4 by using the three equivalent representations given in Eqs. (13).

For each V_4 , *i.e.* for each parameter set

$$\{a_1, a_2, a_3, b_1, b_2, b_3, c_1, c_2, c_3, d_1, d_2, d_3, \epsilon\}, \quad (41)$$

the minimization was repeated multiple times using the procedures above with different random seed points. If any run ever produced a negative value of V_4 , then the minimization cycle would be interrupted, since that negative value definitely means that that V_4 is not BFB. Because Nelder–Mead is relatively fast, it was applied more extensively, in particular over a broader set of field ranges, *i.e.* for $m = 10^5, 10^4, 700, 200, 20, 1$. Differential Evolution usually is more robust, *i.e.* it usually produces a smaller percentage of incorrect results, but it is substantially more expensive; therefore, it was applied only for $m = 10^5, 10^4, 500$.

¹¹Nelder–Mead is a derivative-free optimization method that searches the parameter space by using a simplex. It is not a true global optimization algorithm; nevertheless, in practice it often performs well for problems with a relatively modest number of local minima. Differential Evolution is a population-based stochastic method designed for global optimization. Although computationally expensive, it is relatively robust and tends to work well for problems that have several local minima.

Repeating the minimization with different algorithms, precisions, and initial conditions avoids getting trapped at local minima with steep gradients. Cross-checks of the minimization results indicate that the adopted procedure is highly accurate, albeit computationally quite intensive. In order to ensure reliability and to assess the accuracy of the necessary BFB conditions, we have performed minimization for many data sets, each of them containing one or more millions of quartic potentials.

6 StableWein

6.1 Setup

Installation: StableWein is publicly available at the site

<https://github.com/jurciukonis/StableWein>.

The package may either be installed by cloning the repository

```
git clone https://github.com/jurciukonis/StableWein.git
```

or downloaded directly from the [GitHub repository](#). Once downloaded, the archive should be extracted and the resulting folder (named StableWein) may be placed in a directory chosen by the user. StableWein contains the following components:

- StableWein/StableWein.nb: the main package file;
- StableWein/Binaries/: binary files generated for compiled functions;
- StableWein/Documentation/: documentation files;
- StableWein/Nets/: trained neural networks.

The package may be loaded by evaluating StableWein from any Mathematica session through the command

```
NotebookEvaluate[FileNameJoin[{NotebookDirectory[EvaluationNotebook[]], "WB_package/WB_package.nb"}]]
```

by providing the appropriate path to StableWein.nb.

Compatibility: We verified that StableWein correctly operates with Mathematica versions from 13.2 up to the latest release, viz. 14.3. The package was also tested on Linux, macOS, and Windows operating systems.

StableWein makes use of the Compile function to generate compiled code. In order to enable the option CompilationTarget -> "C", a suitable external C compiler must be installed. Some versions of Mathematica (viz. the 14.x releases) generate compiled functions that execute substantially slower than those produced by earlier versions. In particular, we have observed such performance problems for compiled code containing iterative constructs such as Do, For, Sum and related loop-based operations within Compile. In order to mitigate this problem, we provide the option to load pre-compiled functions generated by using Mathematica 13.2. In order to enable this feature the global boolean variable wbLoadBinaries must be set to True prior to loading the package, i.e. wbLoadBinaries = True.

To improve computational efficiency, we employ global functions instead of local functions. All our global functions are named with a prefix "wb" so that they do not conflict with any other global functions. The same prefix is used in the names of our global variables.

6.2 Package structure

The structure of the package, together with a brief description of the corresponding functionality, is summarized below:

- + `wbWeinUniBFBcheck`: main function for Weinberg model.
 - + **UNI**: implementation of the unitarity constraints.
 - + **Generation**: generation of quartic-potential couplings.
 - **UNI**: filtering of the generated couplings through the UNI constraints.
 - **UNI + NCL1**: filtering of the generated couplings through both the UNI and NCL1 constraints.
 - + **Filtration**: filtering of an imported data set.
 - **UNI**: filtering of couplings through the UNI constraints.
 - + **NNs**: neural network utilities.
 - **Predictions**: prediction of couplings satisfying both the UNI and BFB conditions.
 - **Predictions + validation**: subsequent validation of the predicted data sets by using the selected BFB method(s).
 - + **BFB**: implementation of the BFB constraints.
 - **Sufficient conditions (mode 0)**: application of the sufficient BFB conditions.
 - + **Necessary conditions**: application of the necessary BFB conditions.
 - **Mode 1**: application of the NCL1.
 - **Mode 2**: application of the NCL1, NCL2, and NCL3.
 - **Mode 3**: application of the NCL1, NCL2, NCL3, and NCL4.
 - **Mode 4**: application of brute force to minimize V_4 and find out whether it can ever be negative.
- + `wbBrancUniBFBcheck`: main function for Branco model, with the same sub-items as for Weinberg model, as listed above.

As is evident from the package structure described above, the package has two main entry points: `wbWeinUniBFBcheck`, which selects couplings satisfying the UNI¹² and BFB constraints for Weinberg model, and `wbBrancUniBFBcheck`, which does the same task for Branco model. The internal structure of these two routines is identical. Each of them comprises three main components: (i) verification of the unitarity conditions, (ii) verification of the bounded-from-below conditions, (iii) prediction of viable couplings by using neural networks.

The package may either generate new sets of couplings¹³ or filter imported sets by applying user-selected constraints via the options listed in Table 1. In the generation mode, the couplings are sampled randomly within prescribed ranges and subsequently filtered to satisfy the chosen UNI and/or BFB requirements. Alternatively, neural networks may be used to predict couplings; in this case, the networks predict couplings that satisfy the UNI and BFB constraints simultaneously; the predicted sets of couplings may afterwards, if one so wishes, be validated by using the selected BFB procedures.

The accuracy of the BFB-based filtering is controlled by the choice of mode = 0...4 in the `wbWeinUniBFBcheck` and `wbBrancUniBFBcheck` functions. These functions support a hierarchy of increasingly stringent BFB tests, which trade computational cost for completeness.

¹²These refer to the perturbative unitarity bounds derived in Appendix B.

¹³The generation is done by using a uniform distribution for each coupling within its pre-assigned range. Users who dislike this option must generate their sets of couplings by other means.

Table 1: Options for the functions `wbBrancUniBFBcheck` and `wbWeinUniBFBcheck`.

option	default value	meaning
<code>GeneratePoints</code>	True	generates the initial data set
<code>NPoints</code>	10^3	number of initial points in the data set
<code>MaxCoupling</code>	16	upper bound for each generated coupling
<code>ImposeUNI</code>	True	filters the couplings through the UNI conditions
<code>BoundUNI</code>	8π	unitarity bound (see Appendix B)
<code>ImposeBFB</code>	True	filters the couplings through the BFB conditions defined by set value of mode
<code>NeuralNets</code>	False	uses neural networks
<code>ExportData</code>	False	exports the initial data set and the validated data set to a file
<code>FileNameInit</code>	<code>initial_set.csv</code>	file name for the initial data set
<code>FileNameValid</code>	<code>valid_set.csv</code>	file name for the validated data set
<code>ShowMessages</code>	True	displays messages reporting the computation times and results

Mode 0 corresponds to the sufficient BFB conditions; all the higher modes begin by applying those conditions. This strategy optimizes performance, because quartic potentials that satisfy the sufficient conditions are immediately classified as being BFB; additional checks are required only for potentials that fail the sufficiency test.

In the lowest-accuracy modes, the BFB filter enforces smaller sets of necessary analytic constraints. Higher-accuracy modes incorporate additional necessary conditions, progressively reducing the allowed parameter region. In mode 3, the numerical evaluation relies on a discretized sampling of the relevant orbit-space surface; the sampling resolution may be increased to improve accuracy, at the expense of longer running times. In the most stringent mode 4, `BnessFB` is checked through brute-force numerical minimization of the quartic potential. This provides an explicit cross-check of the necessary conditions implemented in modes 1–3, but with a much longer running time.

Although the package is designed such that users interact mainly with the functions `wbWeinUniBFBcheck` and `wbBrancUniBFBcheck`, all the submodules may also be executed independently by calling the corresponding functions listed in Table 2.

6.3 Usage

We illustrate the use of the package with the function `wbWeinUniBFBcheck`; the function `wbBrancUniBFBcheck` is used analogously. Each of those functions supports two calling patterns:

- `wbWeinUniBFBcheck[mode, options]`,
- `wbWeinUniBFBcheck[list, mode, options]`.

The second pattern uses a data set furnished by the user instead of generating one. Note that the order of the couplings is the one specified in Eq. (41); in Branco model, the generated couplings take the form $\{a_1, a_2, a_3, b_1, b_2, b_3, c_1, c_2, c_3, d_1, d_2, d_3\}$. In both cases, the output is a pair of data sets, where the first one is the initial or generated data set and the second one is the filtered or validated data set. A simple example of using the function would be the command

```
{initParamSet, validParamSet} =  
wbWeinUniBFBcheck[3, "NPoints" -> 10^4, "ExportData" -> True];
```

which generates 10^4 sets of couplings satisfying the UNI conditions, then filters them through BFB mode 3, and exports the validated data sets to a file. Note that `wbWeinUniBFBcheck` does not export the data to files unless instructed to do so; since a variety of data formats may be used, the users are allowed to perform import and export operations in Mathematica as needed. The imported data may be provided to `wbWeinUniBFBcheck` by setting the global parameter `wbParamData`:

```
initFile =  
  Import[FileNameJoin[NotebookDirectory[] <> "/Data/initial_set.csv"  
    ]];  
wbParamData = initFile;  
{initParamSet, validParamSet} = wbWeinUniBFBcheck[3, "GeneratePoints"  
  -> False];
```

Alternatively, the imported data may be passed directly to `wbWeinUniBFBcheck`—in this case,

Table 2: Functions for Weinberg model. For Branco model the functions are analogous and their names have the same structure, but with the substring Wein replaced by Branc.

function	action
<code>wbWeinParRnd</code> , <code>wbWeinParRndNec</code> , <code>wbWeinParRndUni</code> , <code>wbWeinParRndUniNec</code>	generates random, uniformly distributed, couplings of V_4 in the format (41) within different ranges
<code>wbWeinUNICond</code>	filters the couplings through the perturbative unitarity conditions
<code>wbWeinUNINec1Cond</code>	identical to <code>wbWeinParRndUni</code> , but includes additional filtering through the NCL1
<code>wbWeinSufCond</code>	filters the couplings through the sufficient BFB conditions
<code>wbWeinNecCond1</code>	filters the couplings through the NCL1
<code>wbWeinNecCond2</code>	filters the couplings through the NCL1, NCL2, and NCL3
<code>wbWeinNecCond3</code>	filters the couplings through the NCL1, NCL2, NCL3, and NCL4
<code>wbMinimFuncPotWein</code>	minimizes V_4
<code>wbWeinGridGen</code>	auxiliary function for generation of the scanning grid
<code>wbWeinUniBFBcheck</code>	returns couplings satisfying the UNI and BFB constraints with configurable method and accuracy

the option "GeneratePoints" $\rightarrow$ False may be omitted:

```
{initParamSet, validParamSet} = wbWeinUniBFBcheck[initFile, 3];
```

By default, `wbWeinUniBFBcheck` generates an initial data set with the chosen constraints imposed. The number of generated points is controlled by the option `NPoints`. By setting "ImposeUNI" $\rightarrow$ True|False and "ImposeBFB" $\rightarrow$ True|False, one may generate an initial data set that either does or does not satisfy the perturbative unitarity and/or the BnessFB NCL1. The unitarity constraints are described in Appendix B; the moduli of the eigenvalues of the scattering matrices are bounded via the option `BoundUNI`, which is set to 8π by default; if a different unitarity bound is wished for, or if only the BFB constraints are desired, then the range of the generated couplings should be specified by using the option `MaxCoupling`. In particular, a relaxed unitarity bound may be used, e.g.

```
{initParamSet, validParamSet} = wbWeinUniBFBcheck[1, "NPoints"  $\rightarrow$  104,  
"MaxCoupling"  $\rightarrow$  35, "BoundUNI"  $\rightarrow$  16*Pi, "ImposeBFB"  $\rightarrow$  False];
```

Through this command, 10^4 potentials satisfying the UNI conditions with the unitarity bound 16π and with each coupling smaller than 35 in modulus are generated, and no BFB conditions are enforced.

The routine also supports generating viable data sets by using neural network predictions; this is done by setting "NeuralNets" $\rightarrow$ True. The predictors are trained to propose couplings that are expected to satisfy the unitarity and BFB requirements. If "ImposeBFB" $\rightarrow$ True is also set, then the predicted points are additionally validated by using the selected BFB method (modes 1–4); the UNI check is already incorporated into the neural network generation step.

Mode 3 relies on scanning grids that approximate the orbit-space surface represented in Fig. 1. The default grid settings are chosen to be computationally efficient while remaining highly accurate for most practical applications (approximately 99.99% accuracy). The default grid parameters for `wbWeinUniBFBcheck` are `stepsWein` = {17, 40, 0}, whereas for the function `wbBrancUniBFBcheck` the default grid is `stepsBranc` = {17, 15}.¹⁴ In order to further improve the accuracy it may be necessary to increase the grid resolution by raising the integer parameters in `stepsWein` and `stepsBranc` and then applying the function `wbWeinGridGen`:

```
stepsWein = {27, 80, 30};  
{wbfaceListWein, wb\[Theta]ListWein, wb\[Theta]ListWein2}  
= wbWeinGridGen[stepsWein];
```

We warn the user that increasing the grid density may substantially raise the running time of mode 3 filtering while producing only minor changes in the number of accepted potentials.

Maximal accuracy is achieved through mode 4, where quartic potentials in the initial data set are validated through their direct minimization, in accordance with Sec. 5. This mode is useful for checking the BFB-validated points obtained in modes 1–3. We warn the user that the minimization of quartic potentials is computationally expensive and requires substantial computational resources.

¹⁴The list `stepsWein` = { p , r , s }, where p , r , and s are non-negative integers, determines the grid sizes. The integer p specifies the grid used for scanning over the ϖ_k . The finest nominal step is $1/p$; however, the scan includes all the rational values n/m with $1 \leq m \leq p$ and $1 \leq n \leq m$. The integer r defines the grid for the angles ϑ_k , with finest resolution π/r . The integer s controls an additional scan associated with Eq. (26), wherein ϑ_2 is varied with fixed $\vartheta_3 = \pi$ and vice versa. In order to make a finest scan one must increase p and/or r and/or s . The orbit-space surface is sampled in a randomized manner while maintaining an approximately uniform and duplicate-free distribution of points. The grids for the ϖ_k and ϑ_k are computed and stored in memory when the package is loaded; this grid preparation significantly improves the computational efficiency of mode 3 as compared with a direct scan. In the case of Branco model, only two grid parameters are required, viz. { p , r }.

The status of intermediate computations is displayed at the bottom of the evaluation notebook. In addition, messages reporting computation times and results are printed at the end of each step; by setting "ShowMessages" $\rightarrow$ False, these messages are suppressed; this is convenient when `wbWeinUniBFBcheck` is used inside loops or similar workflows. For instance,

```
Table[mode -> Length[Last[wbWeinUniBFBcheck[initParamSet,mode,"
GeneratePoints" -> False,"ShowMessages" -> False]]], {mode,1,4}]
```

We urge the user to check examples in documentation files, which might be the simplest way to get acquainted with the package. The usage messages and documentation files may be accessed by typing a question mark before any function, viz. `?wbWeinUniBFBcheck`.

6.4 Examples

The computations reported in this subsection included four options: both

computations performed for Weinberg model, reported in Table 3;

computations performed for Branco model, reported in Table 4;

and also

computations performed on a desktop computer equipped with an Intel Core i9-13900K CPU (24 cores) and 128 GB of RAM;

computations performed on an Apple MacBook Pro laptop equipped with an M4 Pro CPU (14 cores) and 48 GB of RAM.

All configurations were evaluated under identical conditions, with computations executed in parallel across all available CPU cores. The computations performed on the Intel Core i9 used Mathematica 13.2. Computations performed on the M4 Pro CPU used Mathematica 14.1; in this case and in order to avoid the performance difficulties discussed in Sec 6.1, pre-compiled binaries were used by setting `wbLoadBinaries = True`.

In each one of the four options, we have generated a data set containing 10^6 quartic potentials that satisfy both the unitarity conditions and the BnessFB NCL1.¹⁵ The data sets were then further refined by using both `wbWeinUniBFBcheck` and `wbBrancUniBFBcheck` in the following modes:

- Mode 0: the sufficient BnessFB conditions of Refs. [12] and [13] were applied.
- Mode 2: the necessary BnessFB conditions NCL2 and NCL3, which require no scanning, were applied.
- Mode 3: besides NCL2 and NCL3, the necessary BnessFB condition NCL4, with the default scanning grids of `StableWein`, was applied.
- Mode 3 +: besides NCL2 and NCL3, the necessary BnessFB condition NCL4, with the ameliorated scanning grid +, which is $\{17, 80, 0\}$ for Weinberg model and $\{40, 30\}$ for Branco model, was used.
- Mode 4: the potential was minimized by brute force.

¹⁵The initial data sets were generated by using the pseudo-random uniform distribution implemented in `wbWeinParRndUniNec` and `wbBrancParRndUniNec`. The percentages quoted in Tables 3 and 4 might differ if different distributions were used to generate the initial points.

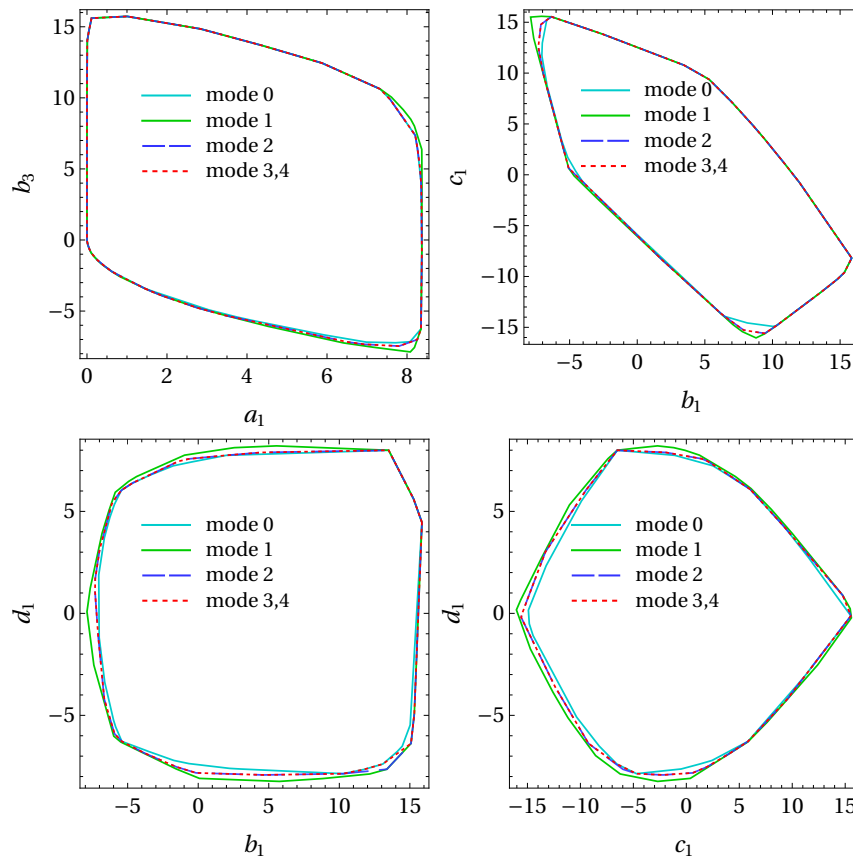


Figure 2: Regions of the parameter space of the Weinberg model that both satisfy the unitarity conditions and pass the BFB constraints at different accuracy modes.

Table 3: Comparison of the results obtained with different computational modes using `wbWeinUniBFBcheck`.

	Intel Core i9			Apple M4 Pro		
	BFB points	Accuracy	Time (s)	BFB points	Accuracy	Time (s)
Generation	1 000 000	—	382	1 000 000	—	533
mode 0	602 536	—	11	600 847	—	4
mode 2	754 471	99.360%	16	753 115	99.361%	7
mode 3	749 674	99.996%	112	748 343	99.995%	559
mode 3 +	749 666	99.997%	693	748 328	99.997%	3747
mode 4	749 640	100%	31 360	748 302	100%	47 961

The accuracy of modes 2 and 3 was assessed by comparing their BFB-accepted potentials with those obtained from brute-force minimization, *viz.* mode 4, according to the formula

$$\text{Accuracy}(\text{mode } i) = \frac{\text{BFB}(\text{mode } 4)}{\text{BFB}(\text{mode } i)} \times 100\%, \quad (42)$$

where $\text{BFB}(\text{mode } i)$ is the number of BFB potentials according to mode i for $i = 2, 3, 4$.

Figure 2 compares the boundaries of the allowed regions obtained for different modes of the BFB constraints, as projected on different two-dimensional planes of parameter space. We

Table 4: Comparison of the results obtained with different computational modes using `wbBrancUniBFBcheck`.

	Intel Core i9			Apple M4 Pro		
	BFB points	Accuracy	Time (s)	BFB points	Accuracy	Time (s)
Generation	1 000 000	—	386	1 000 000	—	529
mode 0	601 644	—	10	602 566	—	4
mode 2	750 018	99.987%	14	751 171	99.990%	8
mode 3	749 925	99.999%	15	751 093	100%	40
mode 3 +	749 923	100%	107	—	—	—
mode 4	749 923	100%	23 941	751 093	100%	36 260

find that, although the sufficient conditions reject nearly 20% of the BFB-allowed points, the corresponding contours in parameter space are only slightly smaller than those obtained from the full BFB test. By contrast, the BFB NCL1 yield slightly larger contours.

6.5 Neural networks

The neural networks were trained to predict the UNI and BFB constraints simultaneously. Because the UNI conditions restrict the allowed ranges of the parameters, the effective training domain is reduced, which improves the attainable predictive accuracy. The neural networks were constructed, trained, and deployed using the capabilities of the Wolfram Language. We employ fully connected feed-forward neural networks with eight layers. In addition, we consider four architectures that differ only in their width, with 2^n neurons per layer for $n = 7, 8, 9, 10$; these architectures are denoted by $\mathbb{N}_7, \dots, \mathbb{N}_{10}$, respectively. The number of layers and neurons was chosen to optimize the trade-off between accuracy and computational efficiency. Based on computational experiments that we have performed, the best performance is obtained with the Ramp activation function and Xavier weight initialization [17].

We found that augmenting the training with synthetic data improves the predictive accuracy. Accordingly, we trained the networks on multiple data sets with different class proportions in order to increase diversity. The first training set was constructed from false samples drawn from the raw data (generated with `wbWeinParRndUniNec` and `wbWeinUNICond`) and supplemented with 20% true samples; the latter were validated through direct minimization of the potential.¹⁶ The two smallest networks, $\mathbb{N}_7^{(1)}$ and $\mathbb{N}_8^{(1)}$, were trained on this data set and subsequently used to generate refined synthetic samples, which were again validated by using the UNI and BFB criteria. Each of the first and second training sets contained 2.5×10^7 samples. All four networks $\mathbb{N}_7^{(2)}$ through $\mathbb{N}_{10}^{(2)}$ were then trained on the second training set.

A third training set was constructed by combining the synthetic samples with the refined, newly generated samples; it contains 5×10^7 entries. All four networks $\mathbb{N}_7^{(3)}$ through $\mathbb{N}_{10}^{(3)}$ were subsequently trained on this third data set. Each network was trained for 500 epochs with a batch size of 2^{14} samples, by using the "RMSProp" optimizer, which adapts the learning rate via an exponentially smoothed estimate of the gradient magnitude. Although large training data sets were used in our study, smaller data sets may be used in practice, since the predictive accuracy improves only marginally when one increases the training-set size.

¹⁶Here, a "true sample" denotes a potential that satisfies both the UNI and BFB conditions, whereas a "false sample" is a potential that violates at least one of those conditions.

We constructed the following neural network chain to classify the potentials:

$$\mathbb{N}_7^{(1)} \rightarrow \mathbb{N}_7^{(2)} \rightarrow \mathbb{N}_7^{(3)} \rightarrow \mathbb{N}_8^{(1)} \rightarrow \mathbb{N}_8^{(2)} \rightarrow \mathbb{N}_8^{(3)} \rightarrow \mathbb{N}_9^{(2)} \rightarrow \mathbb{N}_9^{(3)} \rightarrow \mathbb{N}_{10}^{(2)} \rightarrow \mathbb{N}_{10}^{(3)}, \quad (43)$$

where each subsequent network reclassifies the points accepted by its predecessor. The smaller architectures $\mathbb{N}_7$ and $\mathbb{N}_8$ offer faster inference but lower accuracy when applied directly to raw data, whereas the larger architectures $\mathbb{N}_9$ and $\mathbb{N}_{10}$ achieve higher accuracy at the expense of increased computational cost. Accordingly, combining light-weight and high-capacity networks in the chain (43) yields high overall accuracy while maintaining efficient inference.

StableWein can generate data using NNs by setting "NeuralNets" $\rightarrow$ True in the functions `wbWeinUniBFBcheck` and `wbBrancUniBFBcheck`. If "ImposeBFB" $\rightarrow$ True is additionally specified, then the predicted potentials are further validated by using the selected BFB-accuracy mode. For example, the following command generates a data set of one million points:

```
{initParamSet, validParamSet} =  
wbWeinUniBFBcheck[3, "NeuralNets"  $\rightarrow$  True, "NPoints"  $\rightarrow$  106];
```

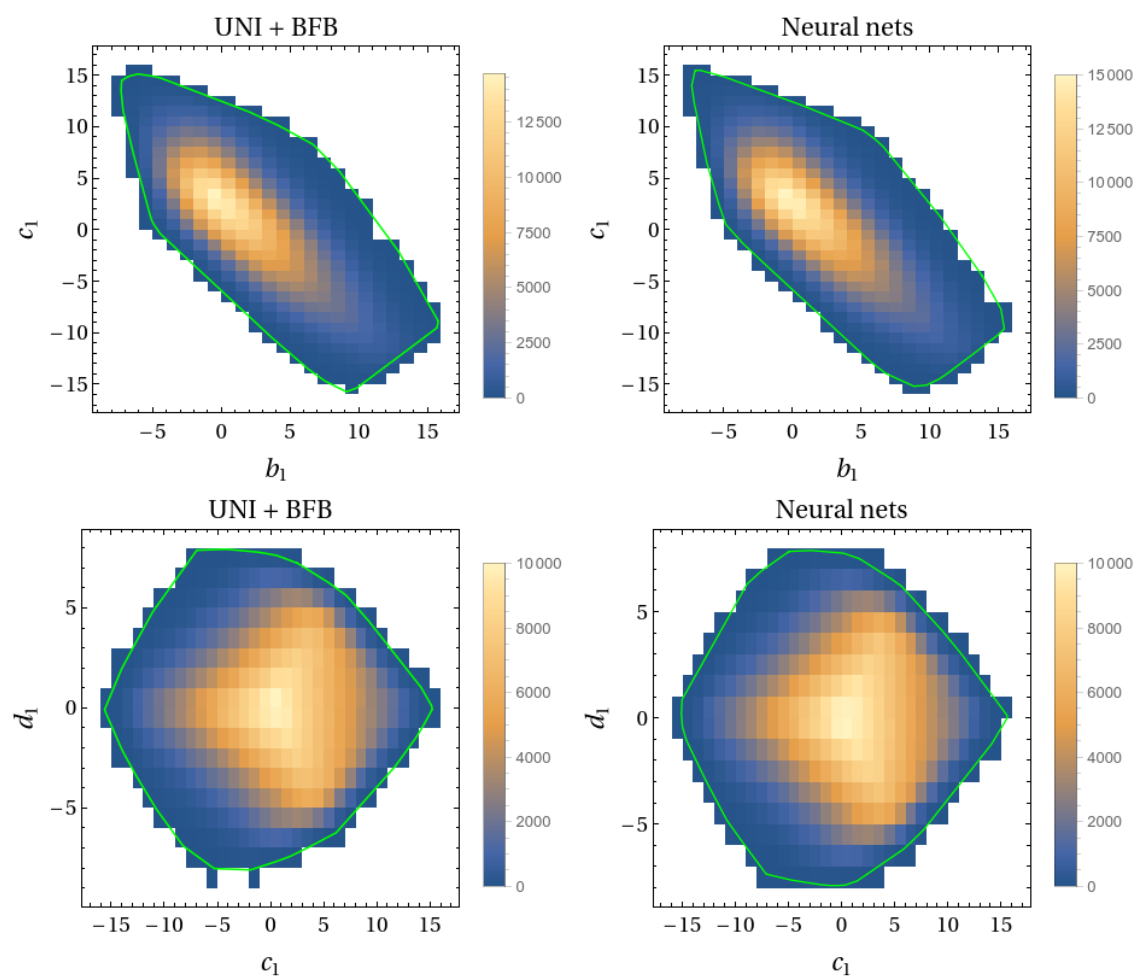


Figure 3: Density histograms of the parameter space in Weinberg model satisfying the UNI constraints and passing the BFB conditions. The left column shows data generated by using `wbWeinUniBFBcheck` with mode 3, while the right column shows data generated by using neural networks.

On a system equipped with an Intel Core i9 processor, generating this data set requires 1 340 s. Enforcing mode 3 yields a neural network prediction accuracy of 99.95%. Although the inference time of the neural network exceeds by one order of magnitude the total running time required both for data generation and subsequent refinement with mode 3 (see Table 3), it still remains one order of magnitude shorter than the time required for direct minimization of the potentials. We also recall that the BFB-filtering times reported in Table 3 correspond to processing only the $\sim 40\%$ of the points that do not satisfy the sufficient conditions.

One may try and adapt the proposed machine learning technique to provide an efficient tool for classifying BFB potentials in models for which neither sufficient nor necessary BFB conditions are known, *e.g.* three-Higgs-doublet models without $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

Figure 3 compares the density of couplings generated by applying the UNI and BFB conditions directly (left panel) to couplings generated by the neural network predictor (right panel). The two two-dimensional projections of parameter space show that the resulting distributions are similar.

It should be noted that on multi-socket systems, *e.g.* workstations and servers, neural network inference may be slower, due to suboptimal thread scheduling and memory-management settings. Such a slowdown of neural network inference was observed by us on a system equipped with an M4 Pro chip.

7 Conclusions

In this work we have analyzed conditions for the scalar potential of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetric three-Higgs-doublet model to be bounded from below (BFB). Rather than striving for sufficient conditions (which select only a portion of parameter space, neglecting potentially physically interesting parts of that space), we argue that, for this model, it is possible to write ever more necessary conditions that progressively approximate the boundary of the BFB region.

As explained in Sec. 5, our computational effort to reliably minimize $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetric 3HDM potentials has allowed us to understand better the boundary separating BFB from non-BFB potentials in parameter space (see, for instance, Fig. 2). By doing so, we were able to compare the accuracy of various necessary conditions. This pursuit culminated in the set of necessary conditions that we call NCL1–4, which can be used to predict, with very high (well above 99%) accuracy, whether a potential is BFB or not, without undue computational effort. Based on our results, we produced and make available the *Mathematica* package *StableWein*, that allows users to predict with varying levels of accuracy whether a $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetric 3HDM potential is BFB, by either generating or inputting a set of quartic couplings.

We have found that the two sets of sufficient conditions of Refs. [12, 13] guarantee that $\sim 60\%$ of randomly generated potentials satisfying UNI and NCL1 are BFB. Conditions (38) guarantee that about 22% of the potentials are BFB, and conditions (34)–(36) do the same for $\sim 60\%$ of the potentials. Still, we have found that neither set of sufficient conditions is a subset of the other one, and we have implemented them both in *StableWein*.

By comparing with numerically minimized sets of quartic potentials (mode 4), we have found that $\sim 75\%$ of the potentials satisfying NCL1 (mode 1) are BFB; moreover, even the simple combination of necessary conditions NCL1–3 (mode 2) achieves close to 99.9% accuracy. The NCL4 (mode 3) requires a scan over the surface of the parameter space represented in Fig. 1; although computationally more expensive than modes 1 and 2, we have found that NCL4 allow one to reach $\sim 99.999\%$ accuracy in scanning potentials for BnessFB. Tables 3 and 4 show that the brute-force numerical minimization used in mode 4 is slower than mode 3 by a factor of $\mathcal{O}(10^3)$ and slower than mode 2 by a factor of $\mathcal{O}(10^4)$, revealing the disproportion between the computational time required for mode 4 and the very high accuracy attained by NCL1–4.

NCL1–4 are computationally less expensive for Branco model. For this reason, instead of treating this model as the particular case of Weinberg model with $\varepsilon = 0$, we have implemented specialized functions to handle Branco model efficiently.

Our necessary conditions are based on reducing the problem of BnessFB to the **strict** copositivity of the matrix in Eq. (15). Consequently, our methods apply only to 3HDM potentials that enjoy $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. The problem of BnessFB of non- $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetric potentials remains untouched.

In addition, the StableWein package provides a neural network option that has been trained to identify BFB $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric potentials. This approach, which relies on neither sufficient nor necessary analytic BFB conditions, achieves good performance, with an accuracy close to 99.9% and fast inference. Consequently, the proposed machine-learning technique can be adapted to classify BFB parameter points in models for which neither sufficient nor necessary BFB conditions are currently available, *viz.* in 3HDM without $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

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A The possible symmetries of a 3HDM

Table 5 gives all the internal symmetries that a three-Higgs-doublet model may have *in the scalar potential alone*.¹⁷ This classification has been systematically developed in Refs. [18–20] (additional details are given in Ref. [21]); a few groups were missed in the classification and were added later [10, 22–25].

The symmetries in Table 5 are the ‘realizable’ ones, *i.e.* the symmetry groups of the potential after any accidental symmetries have been included.

In principle, we should have discarded from Table 5 any subgroup of the $U(1)$ gauge group of hypercharge, because hypercharge is not an *internal* symmetry. A case in point is the group $\mathbb{Z}_3^{\text{center}}$, formed by the transformations (1b) with $\varsigma = 0, 2\pi/3$, and $4\pi/3$. That group is the center of the $SU(3)$ group that mixes the three doublets, which is an internal symmetry, but it is also a subgroup of the $U(1)$ of hypercharge, which is *not* an internal symmetry. Therefore, $U(1)_2$ should rather be written $U(1)_2/\mathbb{Z}_3^{\text{center}}$. On the one hand, for the sake of simplicity, in Table 5 we have omitted writing “ $/\mathbb{Z}_3^{\text{center}}$ ” in all the groups containing $U(1)_2$, and also in $SU(3)$ and $\Delta(54)$. On the other hand, and also for the sake of simplicity, in Table 5 we have used $\Sigma(36)$ instead of $\Sigma(36 \times 3)$ —the latter group includes $\mathbb{Z}_3^{\text{center}}$, and $\Sigma(36) \cong \Sigma(36 \times 3)/\mathbb{Z}_3^{\text{center}}$.

¹⁷We claim neither that these symmetries may be extended to the fermion sector, *viz.* to the Yukawa interactions, nor that the models thus obtained are realistic.

Table 5: Possible symmetries of the scalar potential of a three-Higgs-doublet model. First column: symmetries with $U(1)_1 \times U(1)_2$ subgroup. Second column: symmetries without $U(1)_1 \times U(1)_2$ subgroup but with $\mathbb{Z}_2^{(3)} \times U(1)_2$ subgroup. Third column: symmetries with none of the above subgroups but with $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ subgroup. Fourth column: other symmetries. The symmetries in red produce a scalar potential that automatically enjoys invariance under the CP symmetry $\mathbb{Z}_2^*$; the symmetries in blue lead to a potential that has both a $\mathbb{Z}_2^*$ -invariant version and a CP -breaking one. (*Nota bene*: The potential with both $[\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}] \rtimes \bar{\mathbb{Z}}_2^*$ and $\mathbb{Z}_2^*$ symmetries is the D_4 -invariant one; the potential with both A_4 and $\mathbb{Z}_2^*$ symmetries is the S_4 -invariant one.) The symmetry in green is generated by the ‘generalized CP ’ transformation (A.3).

$U(1)_1 \times U(1)_2$	$\mathbb{Z}_2^{(3)} \times U(1)_2$	$\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$	$\mathbb{Z}_2^{(3)}$
$[U(1)_1 \times U(1)_2] \rtimes S_3$	$D_4 \times U(1)_2$	$[\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}] \rtimes \bar{\mathbb{Z}}_2^*$	$U(1)_2$
$SU(3)$	$O(2) \times U(1)_2$	D_4	$U(1)_1$
$U(2)$		$O(2)$	$\mathbb{Z}_3$
		A_4	$\mathbb{Z}_4$
		S_4	$\mathbb{Z}_2^*$
		$SO(3)$	$\mathbb{Z}_4^*$
			S_3'
			$\Delta(54)$
			$\Sigma(36)$

The symmetry $\mathbb{Z}_2^*$ is the usual CP symmetry generated by

$$\mathbb{Z}_2^*: \quad \Phi_k \rightarrow \Phi_k^*, \quad \forall k = 1, 2, 3. \quad (\text{A.1})$$

The symmetry $\bar{\mathbb{Z}}_2^*$ is the CP symmetry generated by

$$\bar{\mathbb{Z}}_2^*: \quad \Phi_1 \rightarrow \Phi_1^*, \quad \Phi_2 \rightarrow \Phi_3^*, \quad \Phi_3 \rightarrow \Phi_2^*. \quad (\text{A.2})$$

The symmetry $\mathbb{Z}_4^*$ is the CP symmetry generated by

$$\mathbb{Z}_4^*: \quad \Phi_1 \rightarrow \Phi_1^*, \quad \Phi_2 \rightarrow \Phi_3^*, \quad \Phi_3 \rightarrow -\Phi_2^*. \quad (\text{A.3})$$

Many symmetries—the ones in red in Table 5—automatically lead to a scalar potential that is invariant under $\mathbb{Z}_2^*$; other symmetries—the ones in blue—have both a $\mathbb{Z}_2^*$ -invariant version and a $\mathbb{Z}_2^*$ -noninvariant one.

The generators of $U(1)_1$ and $U(1)_2$ are given in Eqs. (1); the generators of $\mathbb{Z}_2^{(3)}$ and $\mathbb{Z}_2^{(2)}$ are given in Eqs. (2) and (3), respectively. The symmetry $\mathbb{Z}_4$ is generated by the transformation

$$\mathbb{Z}_4: \quad \Phi_2 \rightarrow i\Phi_2, \quad \Phi_3 \rightarrow -i\Phi_3, \quad (\text{A.4})$$

which is a particular case of the $U(1)_1$ transformation (1a). The symmetry $\mathbb{Z}_3$ is generated by the transformation

$$\mathbb{Z}_3: \quad \Phi_2 \rightarrow e^{2i\pi/3}\Phi_2, \quad \Phi_3 \rightarrow e^{-2i\pi/3}\Phi_3, \quad (\text{A.5})$$

which is another particular case of the $U(1)_1$ transformation. The symmetry S_3' in the last column of Table 5 has generators (A.5) and

$$\mathbb{Z}_2^{2 \leftrightarrow 3}: \quad \Phi_2 \leftrightarrow \Phi_3. \quad (\text{A.6})$$

The symmetry D_4 is generated by the transformations (2) and (A.6).¹⁸ The symmetry $\Delta(54)$ has generators (A.5), (A.6), and

$$\mathbb{Z}_2^{1 \leftrightarrow 2} : \quad \Phi_1 \leftrightarrow \Phi_2. \quad (\text{A.8})$$

The symmetry S_3 in the first column of Table 5 is generated by the transformations (A.6) and (A.8). The symmetry $\Sigma(36)$ has generators (A.5), (A.8), and

$$\begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix} \rightarrow \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & e^{2i\pi/3} & e^{-2i\pi/3} \\ 1 & e^{-2i\pi/3} & e^{2i\pi/3} \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix}. \quad (\text{A.9})$$

The symmetry A_4 is generated by

$$\mathbb{Z}_2^{(1,2)} : \quad \Phi_1 \rightarrow -\Phi_1, \quad \Phi_2 \rightarrow -\Phi_2, \quad (\text{A.10a})$$

$$\mathbb{Z}_3^{\text{cyclical}} : \quad \Phi_1 \rightarrow \Phi_2 \rightarrow \Phi_3 \rightarrow \Phi_1. \quad (\text{A.10b})$$

The symmetry S_4 is generated by the transformations (A.8) and (A.10).

The symmetry $SO(3)$ is generated by the transformations

$$\begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \rightarrow \begin{pmatrix} \cos \varepsilon & -\sin \varepsilon \\ \sin \varepsilon & \cos \varepsilon \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}, \quad (\text{A.11a})$$

$$\begin{pmatrix} \Phi_2 \\ \Phi_3 \end{pmatrix} \rightarrow \begin{pmatrix} \cos \chi & -\sin \chi \\ \sin \chi & \cos \chi \end{pmatrix} \begin{pmatrix} \Phi_2 \\ \Phi_3 \end{pmatrix}, \quad (\text{A.11b})$$

with arbitrary angles ε and χ . The symmetry $SU(3)$ is generated by the transformations (A.11) and (1). The symmetry $O(2)$ is generated by the transformations (2) and (A.11b). The symmetry $U(2)$ is generated by the transformations (1a) and (A.11b).

The A_4 -symmetric 3HDM has the quartic potential of Eq. (11) with

$$a_1 = a_2 = a_3, \quad b_1 = b_2 = b_3, \quad c_1 = c_2 = c_3, \quad d_1 = d_2 = d_3. \quad (\text{A.12})$$

The S_4 -symmetric 3HDM is A_4 -symmetric and besides has $e^{i\varepsilon} = \pm 1$. The $SO(3)$ -symmetric 3HDM is S_4 -symmetric and besides has

$$a_2 = b_1 + c_1 + d_1. \quad (\text{A.13})$$

The D_4 -symmetric 3HDM also has $e^{i\varepsilon} = \pm 1$ and moreover

$$a_2 = a_3, \quad b_2 = b_3, \quad c_2 = c_3, \quad d_2 = d_3. \quad (\text{A.14})$$

The $O(2)$ -symmetric 3HDM is D_4 -symmetric and obeys Eq. (A.13). The $[\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}] \rtimes \bar{\mathbb{Z}}_2^*$ -symmetric potential obeys Eqs. (A.14) but has free ε .

¹⁸The symmetry $D_4 \times U(1)_2$ should rather be called $[D_4 \times U(1)_2] / [\mathbb{Z}_3^{\text{center}} \times \mathbb{Z}_2^{(2,3)}]$, since the transformation

$$\mathbb{Z}_2^{(2,3)} : \quad \Phi_2 \rightarrow -\Phi_2, \quad \Phi_3 \rightarrow -\Phi_3 \quad (\text{A.7})$$

belongs both to D_4 and to $U(1)_2$. Reference [25] argues that $D_4 \times U(1)_2$ should rather be called $U(1) \circ (\mathbb{Z}_2 \times \mathbb{Z}_2)$.

B Perturbative unitarity bounds (UNI)

In addition to satisfying the BnessFB conditions, the couplings of the quartic part of the potential must remain in a regime where perturbation theory is valid. Only then does the S -matrix admit a controlled expansion in powers of the interaction couplings, thus preserving unitarity. A particular class of theoretical constraints enforcing this requirement arises from the partial-wave decomposition of $2 \rightarrow 2$ scattering amplitudes. These constraints are referred to as partial-wave unitarity bounds.

Consider the $2 \rightarrow 2$ scattering process of scalar fields $AB \rightarrow CD$, with a Lorentz invariant amplitude $\mathcal{M}[AB \rightarrow CD]$. In the center-of-mass frame, we can perform a partial-wave expansion by decomposing the amplitude in the basis of the Legendre polynomials $P_J(x)$ as

$$\mathcal{M}[AB \rightarrow CD] = 16\pi \sum_{J=0}^{\infty} a_J (2J+1) P_J(\cos \theta), \quad (\text{B.1})$$

where θ is the scattering angle, $J = 0, 1, 2, \dots$ is the total angular momentum of the initial/final state, and the numerical coefficients a_J are the partial waves. The orthogonality relations among the $P_J(x)$ allow the partial waves to be determined as

$$a_J = \frac{1}{32\pi} \int_{-1}^{+1} d(\cos \theta) \mathcal{M}[AB \rightarrow CD] P_J(\cos \theta). \quad (\text{B.2})$$

The unitarity of the S -matrix (more specifically the optical theorem) implies that the partial waves must reside within the disk defined by [26]

$$\text{Im } a_J \geq |a_J|^2, \quad \forall J, \quad (\text{B.3})$$

with equality holding for purely elastic processes. The unitarity constraint (B.3) may be rewritten as

$$|a_J| \leq 1, \quad 0 \leq \text{Im } a_J \leq 1, \quad |\text{Re } a_J| \leq \frac{1}{2}, \quad \forall J. \quad (\text{B.4})$$

Let us assume that each partial wave admits an expansion in powers of a coupling λ :

$$a_J = \sum_{n=1}^{\infty} \lambda^n a_J^{(n)}. \quad (\text{B.5})$$

While each full non-perturbative partial wave a_J must satisfy conditions (B.4), a truncated perturbative calculation need not. However, if the partial wave unitarity constraints are not satisfied at tree-level, then higher-order corrections cannot be subdominant, which means that the perturbative expansion is unwarranted. Since tree-level amplitudes are strictly real, it is a necessary condition for the validity of perturbation theory that the tree-level partial waves satisfy

$$|\text{Re } a_J^{(1)}| \leq \frac{1}{2}. \quad (\text{B.6})$$

At tree-level, a $2 \rightarrow 2$ scattering process may have contributions from s , t , and u -channel exchange diagrams, as well as from contact interactions. However, in the ultra-relativistic limit and away from resonances, the Mandelstam variable s becomes large, and then the tree-level amplitude is dominated by the quartic interactions contained in V_4 . In this limit, the scattering amplitude reads

$$\lim_{s \rightarrow \infty} \mathcal{M}[AB \rightarrow CD] = -N_{AB} N_{CD} \frac{\partial^4 V_4}{\partial A \partial B \partial C^* \partial D^*}, \quad (\text{B.7})$$

where $N_{ij} = 2^{-\delta_{ij}/2}$ is a symmetry factor that accounts for identical particles in either the initial state or the final state. Since expression (B.7) is independent of the scattering angle θ , and since $P_0(\cos \theta) = 1$, the strongest perturbative unitarity constraint arises from the zeroth partial wave. Using Eqs. (B.2) and (B.7), the necessary condition (B.6) becomes

$$\left| \operatorname{Re} a_0^{(1)} \right| \leq \frac{1}{2} \quad \Leftrightarrow \quad \left| N_{AB} N_{CD} \frac{\partial^4 V_4}{\partial A \partial B \partial C^* \partial D^*} \right| \leq 8\pi. \quad (\text{B.8})$$

Condition (B.8) is basis-independent, meaning it must be satisfied for *any* linear superposition of initial/final two-particle states. The states in the superposition must have the same quantum numbers under the symmetries of the theory. It is therefore convenient to organize all the states with two scalar fields into coupled-channel scattering matrices, whose entries are given by the corresponding zeroth partial waves in the high-energy limit. For each set of states with the same quantum numbers, perturbative unitarity requires that the *moduli* of the *eigenvalues* of the coupled-channel matrix remain below 8π .

For the $\mathbb{Z}_2^{(3)} \times \mathbb{Z}_2^{(2)}$ -symmetric 3HDM, we label each two-particle state according to

$$\left| Q, Y, T, \mathbb{Z}_2^{(2)}, \mathbb{Z}_2^{(3)} \right\rangle, \quad (\text{B.9})$$

where Q is the total electric charge, Y the total hypercharge, and T the total isospin. As expected, some eigenvalues are identical. The set of two-particle states and the corresponding coupled-channel matrices leading to the minimal set of independent eigenvalues is given by [27]

- $|2, 1, 1, +, +\rangle$: the possible two-particle states are $\{aa, cc, ee\}$, and the corresponding scattering matrix reads

$$\begin{pmatrix} a_1 & d_3 & d_2 \\ d_3 & a_2 & d_1 e^{i\varepsilon} \\ d_2 & d_1 e^{-i\varepsilon} & a_3 \end{pmatrix}. \quad (\text{B.10})$$

- $|2, 1, 1, +, -\rangle$: the only two-particle state is $\{ae\}$, and the corresponding scattering matrix reads

$$(b_2 + c_2). \quad (\text{B.11})$$

- $|2, 1, 1, -, +\rangle$: the only two-particle state is $\{ac\}$, and the corresponding scattering matrix reads

$$(b_3 + c_3). \quad (\text{B.12})$$

- $|2, 1, 1, -, -\rangle$: the only two-particle state is $\{ce\}$, and the corresponding scattering matrix reads

$$(b_1 + c_1). \quad (\text{B.13})$$

- $|1, 1, 0, +, -\rangle$: the only two-particle state is $\{(af - be)/\sqrt{2}\}$, and the corresponding scattering matrix reads

$$(b_2 - c_2). \quad (\text{B.14})$$

- $|1, 1, 0, -, +\rangle$: the only two-particle state is $\{(ad - bc)/\sqrt{2}\}$, and the corresponding scattering matrix reads

$$(b_3 - c_3). \quad (\text{B.15})$$

- $|1, 1, 0, -, -\rangle$: the only two-particle state is $\{(cf - de)/\sqrt{2}\}$, and the corresponding scattering matrix reads

$$(b_1 - c_1). \quad (\text{B.16})$$

- $|1, 0, 1, +, +\rangle$: the possible two-particle states are $\{ab^*, cd^*, ef^*\}$, and the corresponding scattering matrix reads

$$\begin{pmatrix} a_1 & c_3 & c_2 \\ c_3 & a_2 & c_1 \\ c_2 & c_1 & a_3 \end{pmatrix}. \quad (\text{B.17})$$

- $|1, 0, 1, +, -\rangle$: the possible two-particle states are $\{eb^*, af^*\}$, and the corresponding scattering matrix reads

$$\begin{pmatrix} b_2 & d_2 \\ d_2 & b_2 \end{pmatrix}. \quad (\text{B.18})$$

- $|1, 0, 1, -, +\rangle$: the possible two-particle states are $\{cb^*, ad^*\}$, and the corresponding scattering matrix reads

$$\begin{pmatrix} b_3 & d_3 \\ d_3 & b_3 \end{pmatrix}. \quad (\text{B.19})$$

- $|1, 0, 1, -, -\rangle$: the possible two-particle states are $\{ed^*, cf^*\}$, and the corresponding scattering matrix reads

$$\begin{pmatrix} b_1 & d_1 e^{-i\varepsilon} \\ d_1 e^{i\varepsilon} & b_1 \end{pmatrix}. \quad (\text{B.20})$$

- $|0, 0, 0, +, +\rangle$: the possible two-particle states are $\left\{ \frac{aa^* + bb^*}{\sqrt{2}}, \frac{cc^* + dd^*}{\sqrt{2}}, \frac{ee^* + ff^*}{\sqrt{2}} \right\}$ and the corresponding scattering matrix reads

$$\begin{pmatrix} 3a_1 & 2b_3 + c_3 & 2b_2 + c_2 \\ 2b_3 + c_3 & 3a_2 & 2b_1 + c_1 \\ 2b_2 + c_2 & 2b_1 + c_1 & 3a_3 \end{pmatrix}. \quad (\text{B.21})$$

- $|0, 0, 0, +, -\rangle$: the possible two-particle states are $\{(ae^* + bf^*)/\sqrt{2}, (ea^* + fb^*)/\sqrt{2}\}$ and the corresponding scattering matrix reads

$$\begin{pmatrix} b_2 + 2c_2 & 3d_2 \\ 3d_2 & b_2 + 2c_2 \end{pmatrix}. \quad (\text{B.22})$$

- $|0, 0, 0, -, +\rangle$: the possible two-particle states are $\{(ac^* + bd^*)/\sqrt{2}, (ca^* + db^*)/\sqrt{2}\}$ and the corresponding scattering matrix reads

$$\begin{pmatrix} b_3 + 2c_3 & 3d_3 \\ 3d_3 & b_3 + 2c_3 \end{pmatrix}. \quad (\text{B.23})$$

- $|0, 0, 0, -, -\rangle$: the possible two-particle states are $\{(ce^* + df^*)/\sqrt{2}, (ec^* + fd^*)/\sqrt{2}\}$ and the corresponding scattering matrix reads

$$\begin{pmatrix} b_1 + 2c_1 & 3d_1 e^{i\varepsilon} \\ 3d_1 e^{-i\varepsilon} & b_1 + 2c_1 \end{pmatrix}. \quad (\text{B.24})$$

The eigenvalues of the 3×3 matrices (B.10), (B.17), and (B.21) must be determined numerically and then it must be required that their moduli be smaller than 8π . For the remaining matrices, the perturbative unitarity constraints can be written as

$$|b_k| + |c_k| \leq 8\pi, \quad |b_k| + |d_k| \leq 8\pi, \quad |b_k + 2c_k| + 3|d_k| \leq 8\pi, \quad \forall k = \{1, 2, 3\}. \quad (\text{B.25})$$

We have confirmed that both the scattering matrices (B.10)–(B.24) and inequalities (B.25) are in agreement with the results derived in [28].

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