Voyage Across the 2HDM Type-II with Magellan

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Abstract: We review the status of the 2-Higgs Doublet Model (2HDM) Type-II, in the light of the current experimental results and various theoretical consistency conditions. In doing so, we adopt a new numerical framework, called Magellan, to explore the full parameter space of the model. Magellan uses a simple, Markov Chain Monte Carlo technique for the exploration and leverages the use of modern tools, allowing the user to perform inference on the model in an efficient way. The framework exploits the output of well-known Higgs production and decay programs, together with that of packages implementing the current results of both direct and indirect Higgs boson searches. We further illustrate how future measurements can be incorporated in such a framework, through the example of neutral heavy Higgs boson production and decay via the gluon-gluon fusion mode in a variety of final states.

Keywords: 2HDM, Higgs Physics, Parameter Scans, Computing Tools
1 Introduction

The discovery of a Higgs boson at the Large Hadron Collider (LHC) has been a triumph for particle physics [1, 2], revealing that the masses of the fundamental particles in Nature are indeed generated through the Higgs mechanism of (spontaneous) Electro-Weak Symmetry Breaking (EWSB). This particle eventually revealed itself to have properties close to those of the Standard Model (SM) Higgs state. However, even if technically possible, it is rather unnatural thinking that the discovered state would ultimately complete the particle physics scenario. Such a light Higgs state leaves in fact the hierarchy problem unresolved, that is, the great disparity between the Higgs mass itself (125 GeV) and the Planck scale (of order $10^{19}$ GeV).

Under the assumption that the discovered Higgs state is of a fundamental nature, i.e., not a composite state, in order to surpass the hierarchy problem, one has to invoke Beyond the SM (BSM) scenarios that inevitably involve an enlarged Higgs sector. One could have any number of singlet Higgs fields and/or Higgs doublets. Here we consider the presence of a second Higgs doublet, thereby introducing a generic 2-Higgs Doublet Model (2HDM). The presence of a second Higgs doublet can have many other beneficial effects, from both the theoretical and experimental side. From the former perspective, it naturally arises in many models of BSM physics. In the Minimal Supersymmetric Standard Model (MSSM), the existence of two doublets is necessary to generate mass for both up-type and down-type quarks and charged leptons. In this case, the Yukawa couplings should have Type-II values. The representative model chosen in this paper, the 2HDM Type-II, would therefore coincide
with the MSSM in the sparticle decoupling limit. A class of axion models [3, 4], which can explain the lack of observed CP violation in the strong sector, and certain realisations of composite Higgs models with pseudo-Nambu-Goldstone bosons [5–9], both can give rise to an effective low-energy theory with two Higgs doublets. The additional source of CP violation present in this type of enlarged (pseudo)scalar sector could further provide an explanation of the matter-antimatter asymmetry. Particular (modified) realisations of the 2HDM also have the appealing features of being able to explain neutrino mass generation [10], to provide a candidate for dark matter [11] or to accommodate the muon $g - 2$ anomaly [12–14]. From the experimental perspective, the additional four states of a generic 2HDM [15, 16] provide a variety of observables through which the model can be tested.

Hence, it is worthwhile investigating in detail the scope of the LHC in discovering and studying the 2HDM. This is particularly the case for the aforementioned 2HDM Type-II which, in the SUSY context, coincides with the much studied MSSM [15, 17]. However, since there is no evidence of SUSY to date from data, it is appropriate to study the 2HDM Type-II on its own, i.e., assuming that the SUSY scale is much higher than the EW one.

In this pursuit, the standard procedure adopted is to utilise all relevant experimental data and theoretical arguments that can constrain the model. These constraints can be categorised into the following three points:

- Measurements of the discovered 125 GeV Higgs boson properties, such as production and decay signal strengths.
- Direct and indirect searches for the additional companion states present in the model.
- Theory considerations based on perturbativity, unitarity, triviality and vacuum stability.

In this paper, we illustrate how this procedure can be refined in two aspects. On the one hand, we perform an efficient scanning of the parameter space of a BSM scenario through a Markov Chain Monte Carlo (MCMC) approach with T3PS [18]. On the other hand, we also introduce efficient data processing and visualisation methods based on pandas [19], matplotlib [20], bokeh [21] and holoviews [22]. With the help of these packages and the wrapper framework which we nickname Magellan\(^1\), the user can explore the parameter space and the phenomenology of the model with ease.

The plan of the paper is as follows. In Section 2, we describe the 2HDM Type-II, taken as prototypical example to illustrate the described approach. In Section 3, the scanning procedure is specified. Section 4 enumerates the theoretical and experimental constraints that are taken into account during the scan. Section 5 shows how data interpretation is facilitated by these new tools. Finally, in Section 6, we conclude.

\(^1\)Magellan is not published yet. However, a website showcasing interactive dashboards can be accessed via the link given in Ref. [23].
2 The 2HDM

In this section we give a brief introduction to the 2HDM, with a focus on the aspects relevant to our analysis. Extensive reviews of the 2HDM can be found in Refs. [15–17].

An important feature of the model is the number of degrees of freedom (d.o.f) of the fields, which we can be enumerated before and after the spontaneous breaking of the EW symmetry due to the shape of the Higgs potential. Initially, we have two complex doublets, $\Phi_1$ and $\Phi_2$, giving 8 d.o.f. in total. After EWSB, the spectrum contains two CP-even scalars $h$ and $H$, one pseudo-scalar $A$ and two charged Higgs bosons $H^\pm$ (i.e., 5 d.o.f.). The Goldstone bosons of the theory will then become the longitudinal components of the weak $W^\pm$ and $Z$ bosons (3 d.o.f). Hence, the total d.o.f. number is unchanged.

The most general renormalisable (i.e., quartic) scalar potential of two doublets can be written as

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

(2.1)
where $m_{11}^2$, $m_{22}^2$, $m_{12}^2$ are the mass squared parameters and $\lambda_i$ ($i = 1, \ldots, 7$) are dimensionless quantities describing the coupling of the order-4 interactions. Six parameters are real ($m_{11}^2$, $m_{22}^2$, $\lambda_i$ with $i = 1, \ldots, 4$) and four are a priori complex ($m_{12}^2$ and $\lambda_i$ with $i = 5, \ldots, 7$). Therefore, in general, the model has 14 free parameters. Under appropriate constraints, this number can however be reduced.

The potential is explicitly CP-conserving if and only if there exists a basis choice for the scalar fields in which $m_{12}^2$, $\lambda_5$, $\lambda_6$ and $\lambda_7$ are real. Notice that, even in this case, the vacuum could still break CP spontaneously. The spontaneous CP-violation of the vacuum takes place if and only if the scalar potential is explicitly CP-conserving, but there is no basis in which the scalars are real [24]. In the following, we assume that both the scalar potential and the vacuum are CP-conserving. Consequently, by requiring CP-conservation, one loose four d.o.f. reducing the number of free parameters down to 10.

After EWSB, each scalar doublet acquires a Vacuum Expectation Value (VEV) that can be parametrised as follows:

$$\langle \Phi_1 \rangle = \frac{v}{\sqrt{2}} \begin{pmatrix} 0 \\ \cos \beta \end{pmatrix}, \quad \langle \Phi_2 \rangle = \frac{v}{\sqrt{2}} \begin{pmatrix} 0 \\ \sin \beta \end{pmatrix},$$

(2.2)

where the angle $\beta$ determines the ratio of the two doublet VEVs, $v_1$ and $v_2$, through the definition of $\tan \beta = v_2/v_1$. The angle $\beta$ is an additional parameter that adds to the free parameters defining the scalar potential.

In general, the Yukawa matrices corresponding to the two doublets are not simultaneously diagonalisable, which can pose a problem, as the off-diagonal elements lead to tree-level Higgs mediated Flavour Changing Neutral Currents (FCNCs) on which severe
experimental bounds exist. The Glashow-Weinberg-Paschos (GWP) theorem [25, 26] states that this type of FCNCs is absent if at most one Higgs multiplet is responsible for providing mass to fermions of a given electric charge. This GWP condition can be enforced by a discrete $Z_2$-symmetry ($\Phi_1 \rightarrow +\Phi_1$ and $\Phi_2 \rightarrow -\Phi_2$) on the doublets, in which case the absence of FCNCs is natural. The soft $Z_2$-breaking condition relies on the existence of a basis where $\lambda_6 = \lambda_7 = 0$. Therefore, one loses two additional d.o.f. reducing the number of free parameters down to 9. Finally, $m_{11}^2$ and $m_{22}^2$ can be expressed as a function of the other parameters, owing to the fact that the scalar potential is in a local minimum when computed in the VEVs. So, globally, with restrictions to CP-conservation and soft $Z_2$-symmetry breaking, there remain 7 free parameters in the 2HDM.

Under the above conditions, there are several alternative basis in which the 2HDM can be described: the general parametrisation (as given above in terms of $m_{ij}^2$ and $\lambda_i$s), the Higgs basis, where one of the doublets gets zero VEV, and the physical basis, where one uses the physical masses of the scalars. However, in the light of the discovery of the 125 GeV Higgs boson, herein the $h$ state, it is customary to parametrise the theory using the hybrid basis [24], where the parameters provide a convenient choice to give a direct control on both the CP-even and CP-odd Higgs masses, the $hVV$ couplings ($V = W^\pm, Z$), the $Aqq$ vertices and the Higgs quartic couplings. The parameters in this basis are:

\[
\begin{align*}
 m_h, & \quad m_H, & \quad \cos(\beta - \alpha), & \quad \tan \beta, & \quad Z_4, & \quad Z_5, & \quad Z_7. \\
\text{CP-even Higgs masses,} & & \text{determines the} & & \text{ratio of the vevs} & & \text{Higgs self-coupling parameters} \\
\end{align*}
\]

with $m_H \geq m_h$, $0 \leq \beta \leq \pi/2$ and $0 \leq \sin(\beta - \alpha) \leq 1$. The remaining (pseudo)scalar masses can be expressed in terms of the quartic scalar couplings in the Higgs basis:

\[
\begin{align*}
 m_A^2 &= m_h^2 \sin^2(\beta - \alpha) + m_h^2 \cos^2(\beta - \alpha) - Z_5 v_1^2, \\
 m_{H^\pm}^2 &= m_A^2 - \frac{1}{2}(Z_4 - Z_5)v^2.
\end{align*}
\]

In the hybrid basis, by swapping the self-couplings $Z_4$ and $Z_5$ with the scalar masses given above, the 7 free parameters can be recast into four physical masses and 3 parameters.
that are related to the couplings of the scalars to gauge bosons, fermions and scalars themselves, respectively:

\[ m_h, \ m_H, \ m_A, \ m_{H^\pm}, \ \cos(\beta - \alpha), \ \tan(\beta), \ Z_7. \]  

(2.6)

In the above list, \( Z_7 \) enters only the triple and quartic scalar interactions. Finally, as \( m_h \) has been measured with excellent accuracy at the LHC, the number of d.o.f comes down to 6, globally.

Beside the (pseudo)scalar fields, also fermions are required to have a definite charge under the discrete \( Z_2 \)-symmetry. The different assignments of the \( Z_2 \)-charge in the fermion sector give rise to the four different types of 2HDM. The couplings of the neutral Higgses to fermions, normalised to the corresponding SM value (\( m_f/v \), henceforth, denoted by \( \kappa_{hqq} \) for the case of the SM-like Higgs state coupling to a quark \( q \), where \( q = d, u \)), can be found in Tab. 1.

As intimated, in the remainder of this paper, we will concentrate on the 2HDM Type-II. There are two limiting scenarios, giving rise to two distinct regions in the \( (\cos(\beta - \alpha), \ \tan(\beta)) \) parameter plane [27]. They can be understood by examining the behaviour of \( \kappa_{hqq} \) as a function of the angles \( \alpha \) and \( \beta \). Taking the limits \( \beta - \alpha \rightarrow \frac{\pi}{2} \) (upper lines in the upcoming figure) and \( \beta + \alpha \rightarrow \frac{\pi}{2} \) (lower lines in the upcoming figure), the couplings become (recall Tab. 1):

\[ \kappa_{hdd} = -\frac{\sin \alpha}{\cos \beta} = \sin(\beta - \alpha) - \cos(\beta - \alpha) \tan \beta \frac{\beta - \alpha = \frac{\pi}{2}}{\beta - \alpha = 0} 1 \text{ (middle-region),} \]

\[ = -\sin(\beta + \alpha) + \cos(\beta + \alpha) \tan \beta \frac{\beta + \alpha = \frac{\pi}{2}}{\beta + \alpha = 0} -1 \text{ (right-arm),} \]

\[ \kappa_{hua} = \frac{\cos \alpha}{\sin \beta} = \sin(\beta - \alpha) + \cos(\beta - \alpha) \cot \beta \frac{\beta - \alpha = \frac{\pi}{2}}{\beta - \alpha = 0} 1 \text{ (middle-region),} \]

\[ = \sin(\beta + \alpha) + \cos(\beta + \alpha) \cot \beta \frac{\beta + \alpha = \frac{\pi}{2}}{\beta + \alpha = 0} 1 \text{ (right-arm).} \]  

(2.7)

The dependence of \( \kappa_{hdd} \) and \( \kappa_{hua} \) on \( \cos(\beta - \alpha) \) and \( \tan(\beta) \) is illustrated in Fig. 1. The \( \beta - \alpha \rightarrow \frac{\pi}{2} \) case corresponds to the “middle-region”, which is the SM-limit of the theory. In the right-hand side plot of Fig. 1, this domain is identified by the contour region where \( 0.9 \leq \kappa_{hdd} \leq 1.1 \), that is assuming a 10% discrepancy from the SM couplings. The \( \beta + \alpha \rightarrow \frac{\pi}{2} \) case corresponds to the ”right-arm”, where one gets an opposite sign for the coupling between the SM-like Higgs \( h \) and the down-type quarks, relative to the SM value. This is called the wrong-sign Yukawa coupling scenario. In the right-hand side plot of Fig. 1, this region is represented by the narrow arm (or tongue) where the coupling is negative and again has a 10% displacement from the SM value: \( -1.1 \leq \kappa_{hdd} \leq -0.9 \). Both the alignment and the wrong-sign regions are well within the O(10%) discrepancy from the corresponding SM value allowed for the coupling of the SM-like Higgs to the up-type quarks, \( \kappa_{hua} \), as shown in the left-hand plot of Fig. 1.

The most up-to-date 125 GeV Higgs combined signal strength analyses from ATLAS [28] and CMS [29], interpreted in the 2HDM Type-II can be seen in Fig. 2, where it
is found that the hypotheses of $\kappa_{hdd} = 1$ and $\kappa_{hdd} = -1$ are still both allowed. On the theory side, an interesting study [30] based on Renormalisation Group Equations (RGEs) has shown that, if one requires the model to be valid up to higher energies (beyond 1 TeV), the allowed parameter space shrinks to the positive sign of $\kappa_{huu}/\kappa_{hdd}$, otherwise called the alignment region. Below the TeV energy scale, both the alignment and the wrong sign scenario are valid. From a more phenomenological point of view, many analyses have been performed to constrain these two domains. In particular, the importance of the decay channels of the two extra neutral Higgses, $A$ and $H$, in the wrong-sign limit of the model has been clearly illustrated in Ref. [31].

Here, we intend to revisit in detail how the constraints onto the 2HDM Type-II parameter space are normally drawn and whether these can be improved upon. Before doing so, for sake of clarity on the conventions adopted in this paper, in the next section, we describe the tools and framework employed to perform our scans.
Figure 2: Allowed regions of \((\cos(\beta - \alpha), \tan \beta)\) parameters in 2HDM Type-II, obtained from the compatibility with the observed couplings of the 125 GeV boson, when identified as the light Higgs boson, \(h\) of the model. The plot show the most up-to-date available results from ATLAS [28] and CMS [29], seen on the left and right plot respectively.

3 Magellan: global scan for bounds extraction and data interpretation

In this section, we describe the methodology employed to explore the parameter space defined in the previous chapter. The aim of the paper is to illustrate the model exploration approach adopted by Magellan [23], focussing on the 2HDM Type-II. With this new interactive framework, the latest limits on the model are derived.

Magellan is designed for a twofold scope: firstly, to be able to easily import any new experimental results on Higgs measurements and searches so as to interpret these within the 2HDM thus deriving bounds on the parameter space and, secondly, to quickly predict the regions of the latter that can be accessible in a given search with the actual luminosity at hand. The key starting point is implementing all existing constraints, from theory and experiment.

In order to scan over the 2HDM parameter space, we use a MCMC based on T3PS [18] for parallel processing of parameter scans. This tool makes use of the standard Metropolis-Hastings [32, 33] algorithm that is briefly summarised below.

- **Step 0**) Draw a point from the prior distribution \(\pi(\theta)\), which will serve as the starting point of the chain. The likelihood corresponding to this point is \(L(\theta|d)\).

- **Step 1**) Propose a new candidate point \(\theta'\), taken from the proposal distribution \(q(\theta', \theta)\). In our case \(q(\theta', \theta)\) is a Gaussian distribution, centered around the previous point \(\theta\) with a standard deviation of \(a\), commonly referred to as the step-size. The likelihood corresponding to the new point is \(L(\theta'|d)\).
• **Step 2)** Calculate the ratio of the posterior probabilities corresponding to the two points: 
\[ r = \frac{\mathcal{L}(d|\theta')\pi(\theta')q(\theta, \theta')}{\mathcal{L}(d|\theta)\pi(\theta)q(\theta|\theta')}. \]
In the Metropolis-Hastings algorithm, \( q(\theta', \theta) \) is symmetric, therefore it drops out in the ratio.

• **Step 3)** If \( r \geq 1 \), then accept the new proposal, otherwise accept the candidate with a probability of \( r \). If the point is rejected repeat the process from **Step 1**.

• **Step 4)** Once a new candidate is found, add it to chain and repeat the process from **Step 1**.

The likelihood function, \( \mathcal{L}(d|\theta) \), is constructed using the experimental \( \chi^2 \) values coming from the Higgs coupling measurements and the fit to the \( S, T \) and \( U \) parameters of the EW Precision Observables (EWPOs). The likelihood is defined as:

\[
\mathcal{L} = \exp \left( -\frac{\chi^2_{\text{tot}}}{2} \right),
\]  
(3.1)

where \( \chi^2_{\text{tot}} = \chi^2_{\text{HS}} + \chi^2_{ST} \), with \( \chi^2_{\text{HS}} \) being the \( \chi^2 \) value extracted from measurements of the \( h \) couplings entering the production and decays modes of the SM-like Higgs state discovered at CERN (here, we use the output of the program HiggsSignals [34]). The \( S \) and \( T \) parameter compatibility measure (\( U \) is irrelevant for our purposes) \( \chi^2_{ST} \) is:

\[
\chi^2_{ST} = \frac{(S - S^\text{exp}_{\text{best fit}})^2}{\sigma_S^2(1 - \rho_{ST}^2)} + \frac{(T - T^\text{exp}_{\text{best fit}})^2}{\sigma_T^2(1 - \rho_{ST}^2)} - 2\rho_{ST} \frac{(S - S^\text{exp}_{\text{best fit}})(T - T^\text{exp}_{\text{best fit}})}{\sigma_S \sigma_T(1 - \rho_{ST}^2)},
\]  
(3.2)

where the best fit values \( S^\text{exp}_{\text{best fit}} \) and \( T^\text{exp}_{\text{best fit}} \), their uncertainties \( \sigma_S/T \) and the correlation parameter, \( \rho_{ST}^2 \), are taken from the fit result of the Gfitter group [35].

One naturally concentrates on the experimental observables where the discovered \( h \) state enters. However, searches for additional Higgs states, both neutral and charged (at present yielding null results in either case), once interpreted in a specific theoretical model, can force constraints onto its parameter space. Hence, these ought to be included as well. We have done so here using the program HiggsBounds [36].

Another constraint, which must be accounted for, comes from the inclusive weak radiative \( B \)-meson Branching Ratio (BR) that proceeds through the quark-level transition of \( b \to s\gamma \). A recent study [37], using results from the Belle Collaboration, places a 95\% CL lower bound on the charged Higgs mass:

\[ m_{H^\pm} > 580 \, \text{GeV}. \]  

Therefore, we only select points above this mass value.

The algorithm specified above determines how a Markov chain evolves in the parameter space. Since each chain is independent, the different chains can be run in parallel, reducing the wall-clock time of the scan. The MCMC scan is performed over the 6-dimensional parameter space \( (Z_\tau, m_H, m_{H^\pm}, m_A, \cos(\beta - \alpha), \tan \beta) \). The ranges and step-size of each parameter can be found in Tab. 2. Other physical quantities are kept constant and their chosen values are listed in Tab. 3. As the scan is computationally expensive, it is worth specifying what options were chosen for the scan: 400 independent chains were submitted,
Table 2: Range and step-size of the 6-dimensional 2HDM parameters used in the MCMC scan.

| Parameter | min  | max  | step-size |
|-----------|------|------|-----------|
| $Z_7^+$   | −10.0| 10.0 | 0.2       |
| $m_H$ [GeV] | 150  | 1000.0| 20.0      |
| $m_{H^±}$ [GeV] | 500  | 1000.0| 20.0      |
| $m_A$ [GeV] | 100  | 1000.0| 20.0      |
| $\cos(\beta - \alpha)$ | −1.0 | 1.0  | 0.03      |
| $\tan(\beta)$ | 0.5  | 30.0 | 0.5       |

Table 3: Physical parameters kept fixed in our scans.

| $\alpha$ | $\alpha_s$ | $\alpha_{EM} \equiv \alpha(Q^2 = 0)$ | $m_t$ [GeV] | $m_h$ [GeV] |
|----------|------------|-------------------------------------|-------------|-------------|
| 1/127.934 | 0.119      | 1/137.035997                         | 172.5       | 125.09      |

Each for 20 hours on Dual 2.6 GHz Intel Xeon 8 core processor machines. With the given time limit, the setup yields an average chain length of $O(10000)$ steps for each chain. Since the Markov chains first needs to find the minimum of the likelihood, then converge to thermal equilibrium, we account for this “warm-up” period, hence, the first 200 steps are discarded within every chain. The result of the MCMC scan is a data sample consisting of 4,259,823 points, before applying the theoretical constraints (vacuum stability, unitarity and perturbativity). A key feature of the MCMC scanning method is that the results can be interpreted in the Bayesian statistical framework, that is, the density of the points in the parameter space is proportional to the posterior probability of the model describing the data.

A post processing step is then performed where we calculate the production cross-sections and BRs of the (pseudo)scalars using SusHi [38] and 2HDMC [39], respectively. This allows a direct link between experimental measurements and data interpretation within a given BSM theory, like (but not only) the 2HDM Type-II, which is the model we are focussing on in this paper.

4 Bounds on the 2HDM Type-II

In this section, we discuss the bounds that can be extracted on the 6 independent free parameters of the 2HDM Type-II simultaneously taking into account Higgs coupling strength, EWPO and the theoretical constraints.

4.1 Experimental constraints

The values of the EWPOs, $S$, $T$ and $U$ within the 2HDM are derived in [40, 41] and implemented in 2HDMC. The latter depends on the squared masses of the neutral Higgses through the $F$ function [42], which commonly appears in loop calculations:
\begin{align}
F(x, y) &= \frac{x + y}{2} - \frac{xy}{x - y} \ln \frac{x}{y}. \tag{4.1}
\end{align}

$F(x, y)$ is a non-negative function, which is zero for $x = y$, and monotonically increasing with the difference between $x$ and $y$. To simplify the notation, we use $F(A, B)$ denoting $F(m^2_A, m^2_B)$. The $T$ parameter in the 2HDM can be expressed as:

$$
T = c \left\{ \cos^2(\beta - \alpha) \left[ F(H^\pm, h) - F(A, h) - F(H^\pm, H) + F(H, A) \right. \\
+ 3 \left[ F(Z, H) - F(W, H) \right] - 3 \left[ F(Z, h) - F(W, h) \right] \right. \\
\left. + F(H^\pm, H) - F(H, A) + F(H^\pm, A) \right\},
$$

where $c$ is

$$
c = \frac{1}{\alpha_{\text{EM}} \frac{g^2}{64\pi^2 m_W^2}}. \tag{4.3}
$$

In the alignment limit, where $\cos(\beta - \alpha) \approx 0$, the $T$ parameter simplifies to:

$$
T = c \left[ F(H^\pm, H) - F(H, A) + F(H^\pm, A) \right]. \tag{4.4}
$$

From this we see that a mass degeneracy between $A$ or $H$ and $H^\pm$ induces a vanishing $T$ parameter: i.e.,

- $m_{H^\pm} \approx m_H$ implies $T \approx 0$;
- $m_{H^\pm} \approx m_A$ implies $T \approx 0$.
Fixing either $m_H$ or $m_A$ to be equal to the charged Higgs mass is the rule-of-thumb generally taken in the literature to satisfy the EWPO constraints within the 2HDM. However, in the wrong-sign region where $\cos(\beta - \alpha) > 0$, by taking only the leading bound on the $T$ parameter into account, this mass degeneracy can be relaxed to a large extent. This is shown Fig. 3, where we choose the $T$ value to be in the interval: $-0.04 \leq T \leq 0.24$. This choice is based on the GFitter analysis of Ref. [35], where $U = 0$ is imposed for extracting the 95\% CL bounds. As displayed by the orange points, for large $\cos(\alpha - \beta)$ values, that is in the wrong-sign domain, the $m_H$ and $m_A$ masses could simultaneously differ from the charged Higgs mass by roughly 250 GeV (or even more). Very large differences between scalar masses lead to large non-perturbative contributions, though, therefore extreme cases are disfavoured (see later).

The net result, upon including in the MCMC scan the constraints coming from both the SM-like Higgs boson measurements and the EWPOs, is visualised in Fig. 4. There, we plot the allowed points in two parameter planes: $(\cos(\beta - \alpha), \tan \beta)$ (left) as well as $(m_H - m_{H^\pm}, m_A - m_{H^\pm})$ (right). In the first case, we also display the density of points while, in the second case, we split the point between the alignment and wrong-sign scenarios.

4.2 Theoretical constraints

After discussing the limits on the 2HDM Type-II parameter space coming from direct and indirect experimental searches, in this section, we analyse the effect of theoretical constraints. The three major conditions can be concisely summarised as follows.

- Unitarity of the $S$ matrix: the upper bound on the eigenvalues $L_i$ of the scattering matrix of all Goldstone and Higgs 2-to-2 channels [43, 44] is fixed to be

$$|L_i| \leq 16\pi. \quad (4.5)$$

- Perturbativity: the quartic Higgs couplings should be small to justify the perturbative nature of the calculations

$$|\lambda_{H_i H_j H_k H_l}| \leq 8\pi. \quad (4.6)$$

- Stability of the potential: the quartic Higgs potential terms are bounded from below, in turn implying that [45]

$$\lambda_1 > 0, \quad \lambda_2 > 0, \quad \lambda_3 + \sqrt{\lambda_1 \lambda_2} > 0, \quad \lambda_3 + \lambda_4 - |\lambda_5| + \sqrt{\lambda_1 \lambda_2} > 0. \quad (4.7)$$
The general potential coefficients can be expressed with the help of the masses and the angles $\alpha, \beta$ as follows:\(^2\):

\[
\lambda_1 = \frac{m^2_H c^2_\alpha + m^2_\tilde{h} s^2_\alpha - m^2_A s^2_\beta}{v^2 c^2_\beta} - \lambda_5 t^2_\beta - 2\lambda_6 t_\beta, \quad (4.8)
\]

\[
\lambda_2 = \frac{m^2_H s^2_\alpha + m^2_\tilde{h} c^2_\alpha - m^2_A c^2_\beta}{v^2 s^2_\beta} - \lambda_5 s^2_\beta - 2\lambda_7 t^2_\beta, \quad (4.9)
\]

\[
\lambda_3 = \frac{(m^2_H - m^2_\tilde{h}) s_\alpha c_\alpha + (2m^2_H + m^2_A) s_\beta c_\beta}{v^2 s^2_\beta c^2_\beta} - \lambda_5 - \lambda_6 s_\beta - \lambda_7 t_\beta, \quad (4.10)
\]

\[
\lambda_4 = \frac{2(m^2_A - m^2_H)}{v^2} + \lambda_5, \quad (4.11)
\]

\[
\lambda_4 - |\lambda_5| = \frac{2(m^2_A - m^2_H)}{v^2} + \lambda_5 - |\lambda_5| = \begin{cases} \frac{2(m^2_A - m^2_H)}{v^2}, & \text{if } \lambda_5 > 0, \\ \frac{2(m^2_A - m^2_H)}{v^2} - 2|\lambda_5|, & \text{if } \lambda_5 > 0. \end{cases} \quad (4.12)
\]

Out of these, the stability and the perturbativity of the potential pose the most severe constraints on the parameter space. In order to give an overview of the bounds coming from the theoretical constraints, in Fig. 5, we display the 2HDM Type-II parameter space regions excluded by the different sources. For illustrative purposes, we have fixed the mass of the (pseudo)scalars to be $m_{H^\pm} = 600$ GeV and $m_A = 300$ and 400 GeV. The blue dots reflect the bounds arising from the requirement of unitarity. The effects are concentrated in the medium-high $\tan \beta$ range and for $|\cos(\beta - \alpha)| \geq 0.1$. Positive(negative) values

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\(^2\)Hereafter, we use the notation $c_X, s_X$ and $t_X (X = \alpha, \beta)$ to signify $\cos X, \sin X$ and $\tan X$, respectively.
Figure 5: Distribution of the parameter space points on the \((\cos(\beta - \alpha), \tan \beta)\) plane excluded by the theoretical constraints of unitarity (blue hollow dots), perturbativity (magenta hollow squares) and stability (black crosses) in the 2HDM Type-II. The masses of the heavy Higgs, \(H\) and the charged Higgs \(H^\pm\) are fixed at \(m_{H^\pm} = m_H = 600\) GeV. The HiggsSignals and EWPO allowed regions correspond to the yellow, green, blue regions, with 1, 2 and 3\(\sigma\) CL compatibility respectively. The points excluded by HiggsBounds are also shown as red crosses.

of \(Z_7\) disfavour the negative(positive) values of \(\cos(\beta - \alpha)\), shifting the excluded region on the right-(left-)hand side. The unitarity bounds do not affect the alignment and the wrong-sign domains, allowed by the HiggsSignals and EWPO constraints and represented by the blue(green and yellow) region at the 95\% (90\% and 68\%) CL. The perturbativity constraint, represented by the magenta squares, extends the excluded region towards lower values of \(\tan(\beta)\) and \(|\cos(\beta - \alpha)|\) for the chosen value of the quartic Higgs coupling. The effect of \(Z_7\) is the same as for unitarity. Finally, the stability of the potential, represented by the black crosses, excludes all the negative values of \(\cos(\beta - \alpha)\) and part of the positive values so to suppress almost completely the alignment domain. A very few allowed points lie in the alignment region at extremely low \(\tan \beta\) values, while the majority is concentrated
in the wrong-sign domain. By increasing the $m_A$ value, the alignment and the wrong-sign scenarios get both populated again.

The conclusion to be drawn from this exercise is that the stability of the scalar potential enforces a lower bound on the pseudoscalar mass, $m_A$, in the alignment portion of the parameter space. We analyse this effect in more details in the next section.

### 4.3 The role of $m_A$

In this subsection we investigate the conditions imposed by a stable scalar potential and their effect on the two limits of the model under consideration (2HDM Type-II): the alignment and wrong-sign domains. We use a collection of points from the MCMC scan, which passes the condition $\Delta_{\chi^2}^{\text{tot}} < (3\sigma \text{ CL upper limit})$ without imposing any other constraints. The stability inequalities in Eq. (4.7) are implemented step-by-step to be able to uniquely identify their effect on the parameter space. The following observations can be made.

- At the beginning (without imposing any of the stability conditions) there are points present in both the alignment and wrong-sign limit regions.
- The constraints $\lambda_1 > 0$ and $\lambda_2 > 0$ are targeting points from both regions irrespectively of the $m_A$ value.
- There are surviving points in both regions after imposing $\lambda_1 > 0$ and $\lambda_2 > 0$.
- The condition $\lambda_3 + \sqrt{\lambda_1 \lambda_2} > 0$ does not exclude any additional points for low $m_A$ values but discards a large number of points exclusively from the alignment limit in the high $m_A$ domain.
- The final constraint of $\lambda_3 + \sqrt{\lambda_1 \lambda_2} + \lambda_4 - |\lambda_5| > 0$ again disfavours points from the alignment region independently on the $m_A$ value. More importantly, this proves to exclude all of the points from the alignment limit region in the low-intermediate $m_A$ range, with the exception of a handful of points at low $\tan \beta$. Contrary to this, the high $m_A$ range contains surviving points in both regions after imposing all the conditions.

This result is visualised in the scatter plots of Fig. 6, where we display the $(m_H, m_A)$ parameter space. The blue dots represent the alignment region while the red ones refer to the wrong-sign scenario. In these plots, we enforce the experimental bounds coming from HiggsSignals and EWPOs plus the theoretical constraints discussed above. We moreover set the lower bound on the charged Higgs mass at 600 GeV. In the left plot, one can see that very few points are left in the alignment region at low $m_A$. Those few are characterised by very small values of $\tan \beta$, as discussed previously. If we superimpose the HiggsBounds limits, even these remaining points disappear.

The global picture is shown in the right plot of Fig. 6. There one can see that, in the alignment limit of the 2HDM, the pseudoscalar state is required to be rather heavy: $m_A \geq 350$ GeV. Only in the wrong-sign scenario, it can in principle have a mass as light as $m_A \simeq 150$ GeV (see red dots), when $Z'_7$ is rather large and positive definite as shown in Fig. 5. This latter feature is the result of the effects coming from the perturbativity enforcement.
This picture depends however on the limit that could be in future set on the charged Higgs mass. Raising the $m_{H^\pm}$ limit pushes the lower bound on $m_A$ further up, in the alignment scenario. In the wrong-sign domain, one can still have light CP-odd Higgs masses at the price of stretching $Z_7$ towards large and positive values, $Z_7 \geq 1$, typically. This is in agreement with the findings given in Ref. [46]. Here, we have added a more detailed analysis of the effects coming from the individual constraints, highlighting in particular the role of the stability requirement on the scalar potential in setting a lower bound on the CP-odd Higgs mass in the alignment scenario.

In this section, we have described framework and tools to extract the portion of the 2HDM Type-II parameter space that is allowed by the present experimental constraints (summarised by HiggsSignals, EWPOs and HiggsBounds) and the theoretical requirements. We are now ready to discuss the possibilities that Magellan, the global scan tool we are presenting in this paper, offers to interpret the LHC data coming from a variety of up-to-date analyses within this specific model we are focussing on, the 2HDM Type-II.

5 Data interpretation

In this chapter, we apply the methodology of the global scan tool, Magellan, to interpret the LHC data within the 2HDM Type-II. During the course of the MCMC scan, various experimental and theoretical properties linked to the individual parameter space points are computed and saved. This retained information allows to examine different aspects of the model from the same dataset. Any new unfolded experimental results can be then translated into direct bounds on the parameter space of the BSM scenario at hand, the 2HDM Type-II. The experimental results corresponding to a given observable, typically the 95% CL exclusion bound on the cross-section times BR, can be projected onto any two-dimensional sections of the full parameter space, thus allowing the extraction of limits
on different parameters of the theory. The observables, i.e. cross-sections and BRs used for comparison, are computed by making use of SusHi and 2HDMC.

As a working example, in the following, we consider the most recent ATLAS analysis of the process $pp \to A \to Zh \to Zb\bar{b}$ [47]. The search for the heavy CP-odd Higgs, $A$, decaying into a $Z$ boson and the 125 GeV Higgs state, is performed by looking at final states with either two opposite-sign charge leptons ($l^+l^-$ with $l = e, \mu$) or a neutrino pair ($\nu\bar{\nu}$) plus two $b$-jets at the 13 TeV LHC with a total integrated luminosity of $L = 36.1$ fb$^{-1}$. The 95% CL upper bound on the cross-section times BR as a function of the CP-odd Higgs mass $m_A$ is shown in the left plot of Fig. 7. There, it is assumed that the possible signal comes from the pure gluon-gluon fusion production. In the right plot of the same figure, the theoretical cross-section times BR is computed within the 2HDM Type-II for the same $m_A$ range. The different colours of the scatter points correspond to the values of $\cos(\alpha - \beta)$ shown in the top-right legend. The cross-section times BR depends on this parameter, sensibly. The couplings of the CP-odd Higgs, $A$, with the heavy quarks in the production subprocess and with the $Z$ and $h$ bosons in its subsequent decay all depend on $\cos(\alpha - \beta)$. Superimposed on this scatter-plot, there are the observed and expected curves taken from the ATLAS analysis (see left plot). From direct comparison, one can immediately see the excluded range of the CP-odd Higgs mass as a function of the $\cos(\alpha - \beta)$ value. This comparison can be further extended by taking into account the limit on the cross-section expected in a near future with a luminosity $L = 300$ fb$^{-1}$. The projected exclusion bounds on the $\cos(\alpha - \beta)$ show indeed a sensible improvement.

Beyond this, Magellan allows the extraction of a rich variety of information. The toolbox leverages the use of the DataFrame class of pandas, making a custom selection

![Figure 7](image-url)
Figure 8: Projections of the 2HDM Type-II parameter and observables. The blue points are those allowed by HiggsSignals, EWPOs and theoretical constraints. The red ones are those excluded by the ATLAS analysis of the process $pp \rightarrow A \rightarrow Zh \rightarrow Zb \bar{b}$ with a luminosity of $L = 36.1 \text{ fb}^{-1}$.

on the set of points relatively easy. Excluded (or allowed) points by a given theoretical constraint or experimental bound can then be projected onto any other plane, defined by the desired choice of model parameters or observables. In the specific case mentioned above, one can select points above the 95\% CL upper bound on the observed cross-section times BR, given by the black solid line on the right plot of Fig. 7, and project those points in order to see the effect of that particular model-independent measurement on all the free parameters of the 2HDM Type-II. Note that, as the limits coming from the experimental analyses reported on HEPData (https://www.hepdata.net/) depend on the assumption made on the width of the new hypothetical Higgs bosons, when involved, the width of the (pseudo)scalar states is equally taken into account when extracting the bounds on the parameter space.

This feature is sketched in Fig. 8. Nine different 2D projections of model parameters and observables are shown, where first the points excluded by the analysis (red) are drawn,

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Experimental limits are available up to $\Gamma_A/m_A < 11\%$. 
and then non-excluded points (blue), indicating the region of the parameter space on 2D planes which are likely to be excluded, irrespective to the other hidden parameters. One could also choose to visualise the results in the opposite order, that is first the non-excluded points and then the excluded ones. In this way, the region of the parameter space tested by the specific experimental measurement at hand would stand out. The double option is implemented and shown on the Magellan interactive webpage [23].

From this subgroup of possible parameter spaces, one can already conclude that the low $\tan \beta$ region is the one being tested, i.e., $\tan \beta \leq 5$ (c.f. the (cos($\beta - \alpha$), $\tan \beta$) plane). There the range cos($\beta - \alpha$) $\geq$ 0.5 is almost excluded for all $m_A$ masses (c.f. the (cos($\beta - \alpha$), $m_A$) projection). Thus, even if initially one built a colourless scatter plot of the $pp \to A \to Zh \to Zb\bar{b}$ rate as a function of $m_A$, with no information on the cos($\beta - \alpha$) value of the individual points, the projection feature could shed light on the range of cos($\beta - \alpha$) and $\tan \beta$ that one is testing.

Also, by looking at the top-right plot showing the value of the width of the CP-odd
Higgs over its mass as a function of $\cos(\beta - \alpha)$, one can see that the present analysis covers a parameter space up to where $\Gamma_A/M_A \leq 11\%$. But the possible values of this ratio extend up to $\Gamma_A/M_A \simeq 25\%$. This would imply that future experimental analyses should stop relying on the pure narrow width approximation and diversify their approach to include the search for wider resonances.

Projecting the points excluded by the expected limit on the production cross-section times BR of the process $pp \to A \to Zh$, at an integrated luminosity of $L = 300 \text{ fb}^{-1}$, on the same projection planes as Fig. 8, one can see that a very significant portion of the parameter space could be under scrutiny. This is shown in Fig. 9 by the red scatter points. The region $\cos(\beta - \alpha) \geq 0.4$ could already be excluded, as shown by the top-right and bottom-left plots. Also the alignment region would start to disappear. This already gives a rather good idea of what will happen in the next data taking stages at the LHC.

This way of interpreting the model-independent experimental data within a given model is much more flexible and complete than the procedures adopted in the literature. Referring in particular to the most recent $pp \to A \to Zh$ search performed by ATLAS [47], one can notice that, for the interpretation of the cross-section times BR limits in the context of the 2HDM, the $H^\pm$, $H$ and $A$ bosons are assumed to be degenerate. In our analysis, the three masses can differ by 250 GeV and more, as detailed in Section 4.1. Moreover, the visualisation of the limits at 95\% CL on the 2HDM parameters as given in Ref. [47] is constrained and therefore partial. Bounds are in fact displayed on the $(\tan\beta, \cos(\beta - \alpha))$ plane, at a fixed value of the resonance mass $m_A$, and on the $(\tan\beta, m_A)$ plane, at a fixed value of $\cos(\beta - \alpha)$. The global scan presented in this paper can go beyond these limitations and display the full limits on any 2D plane, offering access to a rich variety of information.

5.1 2HDM sensitivity of different measurements at the LHC

In this section, we analyse different possible measurements that can be performed at the LHC with the aim to show their sensitivity to a given set of model parameters within the 2HDM Type-II. We discuss first the relevance of the various channels, which might contain one or more Higgses as intermediate states, in covering portions of the parameter space via the study of the BRs of the CP-odd $A$ and the CP-even (heavy) $H$. Some of these portions show a partial overlap, some others are disjoint, as displayed in Fig. 11.

There, by looking at the top row, one can clearly see that the $A \to t\bar{t}$ (red) and $A \to ZH$ (light blue) channels are quite complementary. The first one is sensitive to low $\tan\beta$ values (see top-left plot) and can cover a broad range of the mass spectrum where the $A$ and $H$ masses do not differ more than 200 GeV from each other and no hierarchy between them is made explicit (see top-right plot). On the contrary, the latter becomes relevant for low to medium $\tan\beta$ values and when an explicit hierarchy is in place. The $A$ decay into down type particles, $b$-quarks or $\tau$-leptons, is enhanced at medium-to-high values of $\tan\beta$, as displayed by the green and yellow points in the top-left plot. Finally, the $A \to Zh$ mode is particularly sensitive to the large $\cos(\beta - \alpha)$ region and low to medium $\tan\beta$ values. If we instead look at the $H$ decay modes (see bottom row), we see that they are dominated by the decays into $b\bar{b}$, $\tau^+\tau^-$ at high $\tan\beta$ and $t\bar{t}$, $ZA$ at low $\tan\beta$. These decays are concentrated in the alignment region. This means that the processes mediated
by the heavy $H$ scalar are not sensitive to the region of large $\cos(\beta - \alpha)$. For probing or excluding this portion of the parameter space, that is, the wrong-sign scenario, one needs to rely on processes mediated by the $A$ state, in particular $A \rightarrow Zh$.

The decay modes give of course only a partial picture of the sensitivity of the experimental searches to the free parameters of the theory. One should consider the total rate, that is, production cross-section times BR(s), in order to have a complete view. This is displayed in Fig. 10, where we plot the gluon-gluon induced cross-section for the CP-odd Higgs in the bi-dimensional $(\cos(\beta - \alpha), \tan \beta)$ plane, and in Fig. 12, where we display the same observable for the heavy CP-even Higgs mediated processes. The magnitude of the total cross-section is given following the colour code on the right columns. For the $A$ mediated processes, the cross-section can range from the order of 30 pb, corresponding to $gg \rightarrow A \rightarrow t\bar{t}$, to the order of a few fb, corresponding to the $\tau^+\tau^-$ channel. Analogous results hold for the $H$ mediated processes.

6 Summary

In this paper, we have tensioned the 2HDM Type-II against data stemming from a variety of experimental contexts. We have included a wide range of results spanning from the old high precision LEP and SLC data, encoded into the so-called EWPOs, to the latest...
measurements performed at the LHC. This was done to assess whether the enlarged Higgs sector embedded in such a construct has survived experimental scrutiny to date and can thus be taken as a solid theoretical framework in which searches for new Higgs signals can be pursued at the LHC in the near future. In particular, we have shown that two distinct configurations of the parameter space of the 2HDM Type-II are currently compliant with all such data and also satisfy internal consistency requirements of the model, namely, the so-called ‘wrong-sign’ scenario (up to 1 TeV scale) and the ‘alignment’ limit.

Both of these can be probed during the upcoming runs of the LHC. The dynamics enabling one doing so are the production channels $pp \rightarrow A$ and $pp \rightarrow H$, i.e., those yielding, respectively, the heavy CP-even and CP-odd Higgs states belonging to the 2HDM Type-II spectrum. These extra Higgs bosons can in turn decay into a variety of modes, including chain decays of one Higgs boson into another, e.g., $A \rightarrow Zh$ and $H \rightarrow ZA$. These processes contain all the neutral Higgs bosons of such a BSM scenario ($h$ represents the discovered SM-like Higgs state). The sensitivity of future LHC stages to all such production and decay modes was studied and it was argued that a combination of these could potentially pave

**Figure 11:** Top plots: regions of the two-dimensional parameter spaces with high BRs of the CP-odd Higgs, $A$, in the channels given in the legend of the top-left plot. Bottom plots: same for the heavy CP-even Higgs, $H$, decaying into the channels listed in the legend of the bottom-left plot.
Figure 12: Magnitude of the total cross-section times BR in the \((\cos(\alpha-\beta), \tan \beta)\) plane for four different processes mediated by the heavy CP-even Higgs, \(H\). From top-left to bottom-left (clock-wise): \(pp \rightarrow H \rightarrow ZA\), \(pp \rightarrow H \rightarrow AA\), \(pp \rightarrow H \rightarrow t\bar{t}\) and \(pp \rightarrow H \rightarrow \tau^-\tau^+\).

the way to the detection of all such neutral states of the 2HDM Type-II. In particular, the discovery of a low-mid mass CP-odd Higgs boson, \(m_A \leq 400\) GeV, could exclude the alignment limit of the 2HDM Type-II.

This conclusion was achieved by exploiting the unique technical features of a new numerical framework called Magellan. The framework is based on a MCMC exploiting the Metropolis-Hastings algorithm (via T3PS) which features the following key elements: use of parallel processing when doing parameter scans, efficient data storage with fast I/O and interactive visualisation. Further, it can be linked to external packages enabling one to test theoretical models against experimental data (such as HiggsBounds and HiggsSignals) as well as to those enabling the prediction of the Higgs production and decay observables used for this purpose (such as SusHi and 2HDMC). We have demonstrated some of its capabilities in relation to the mapping of the present and future LHC sensitivity to the aforementioned dynamics of the 2HDM Type-II.

We have therefore equipped ourselves and readers with the ideal framework to test the hypothesis of an enlarged Higgs sector existing in Nature, as the Magellan voyage undertaken here can easily be repeated into other BSM frameworks.
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