Analysis of an extended scalar sector with $S_3$ symmetry

Dipankar Das$^1$, Ujjal Kumar Dey$^2$

$^1$Saha Institute of Nuclear Physics, 1/AF Bidhan Nagar, Kolkata 700064, India
$^2$Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Allahabad 211019, India

Abstract

We investigate the scalar potential of a general $S_3$-symmetric three-Higgs-doublet model. The outcome of our analysis does not depend on the fermionic sector of the model. We identify a decoupling limit for the scalar spectrum of this scenario. In view of the recent LHC Higgs data, we show our numerical results only in the decoupling limit. Unitarity and stability of the scalar potential demand that many new scalars must be lurking below 1 TeV. We provide numerical predictions for $h \rightarrow \gamma\gamma$ and $h \rightarrow Z\gamma$ signal strengths which can be used to falsify the theory.

1 Introduction

The newly observed boson at the Large Hadron Collider (LHC) [1, 2] fits very well to the description of the Higgs scalar in the Standard Model (SM). The SM relies on the minimal choice that a single Higgs doublet provides masses to all particles. But unexplained phenomena like neutrino masses and existence dark matter motivate us to contemplate other avenues beyond the SM (BSM). Majority of these BSM scenarios extend the SM Higgs sector predicting a richer scalar spectrum. One of them – the $S_3$ flavor model – stems from an effort to answer the aesthetic question as to why there are precisely three fermion generations [3]. Keeping the fermions in appropriate $S_3$-multiplets, it is possible to reproduce all the measured parameters of the CKM and PMNS matrices as well as make testable predictions for the unknown parameters of the PMNS matrix [4–24]. But one needs at least three Higgs doublets to achieve this goal [6]. However, the $S_3$ invariant scalar potential contains some new parameters which are difficult to constrain phenomenologically. Although some lower bounds on the additional scalar masses can be placed from the Higgs mediated flavor changing neutral current (FCNC) processes [25], these bounds rely heavily on the Yukawa structure of the model. In this article we will present some new bounds on the physical scalar masses which do not depend on the parameters of the Yukawa sector.

To achieve this, we will employ the prescription of tree unitarity which is known to be able to set upper limits on different scalar masses [26]. Although various aspects of the $S_3$ scalar potential have been discussed in the literature [27,28], to the best of our knowledge, this is the first attempt to derive the exact unitarity constraints on the quartic couplings in the $S_3$ invariant three-Higgs-doublet model (S3HDM) scalar potential. We also identify a decoupling limit in the context of S3HDM where a CP-even Higgs with SM-like properties can be obtained. Since the recent LHC Higgs data seem to increasingly leaned towards the SM expectations, our numerical analysis will be restricted to this limit.

The paper is organized as follows : in Section 2 we discuss the scalar potential and derive necessary conditions for the potential to be bounded from below. In Section 3 we minimize the potential and calculate the physical scalar masses. In this section we also figure out a decoupling limit in which one neutral CP-even physical scalar behaves exactly like the SM Higgs. In Section 4 we derive the exact constraints arising from the considerations of tree level unitarity and use them to constrain the nonstandard scalar masses. In Section 5 we quantitatively investigate the effect of the charged scalar induced loops on $h \rightarrow \gamma\gamma$ and $h \rightarrow Z\gamma$ signal strengths. Finally, we summarize our findings in Section 6.

1 d.das@saha.ac.in
2 ujjaldey@hri.res.in
\section{The scalar potential}

$S_3$ is the permutation group involving three objects, $\{\phi_a, \phi_b, \phi_c\}$. The three dimensional representation of $S_3$ is not an irreducible one simply because we can easily construct a linear combination of the elements, $\phi_a + \phi_b + \phi_c$, which remains unaltered under the permutation of the indices. We choose to decompose the three dimensional representation into a singlet and doublet as follows:

\begin{align}
1 : \quad & \phi_3 = \frac{1}{\sqrt{3}}(\phi_a + \phi_b + \phi_c), \quad (1a) \\
2 : \quad & \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix}(\phi_a - \phi_b) \quad \begin{pmatrix} 1 \\ \sqrt{6} \end{pmatrix}(\phi_a + \phi_b - 2\phi_c). \quad (1b)
\end{align}

The elements of $S_3$ for this particular doublet representation are given by:

\begin{align}
&\begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}, \quad \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}, \quad \text{for} \quad \left( \theta = 0, \pm \frac{2\pi}{3} \right). \quad (2)
\end{align}

The most general renormalizable potential invariant under $S_3$ can be written in terms of $\phi_3, \phi_1$ and $\phi_2$ as follows $[27-31]$:

\begin{align}
V(\phi) &= V_2(\phi) + V_4(\phi), \\
\text{where,} \quad V_2(\phi) &= \mu_1^2(\phi_1^+ \phi_1 + \phi_2^+ \phi_2) + \mu_2^2 \phi_3^+ \phi_3, \\
V_4(\phi) &= \lambda_1(\phi_1^+ \phi_1 + \phi_2^+ \phi_2)^2 + \lambda_2(\phi_1^+ \phi_2 - \phi_2^+ \phi_1)^2 + \lambda_3 \left\{ (\phi_1^+ \phi_2 + \phi_2^+ \phi_1)^2 + (\phi_1^+ \phi_1 - \phi_2^+ \phi_2)^2 \right\} \\
&\quad + \lambda_4 \left\{ (\phi_1^+ \phi_1)(\phi_2^+ \phi_2) + (\phi_2^+ \phi_2)(\phi_1^+ \phi_1) + (\phi_1^+ \phi_1)(\phi_2^+ \phi_2) + \text{h.c.} \right\} \\
&\quad + \lambda_5 (\phi_1^+ \phi_1)(\phi_2^+ \phi_2) + \lambda_6 \left\{ (\phi_3^+ \phi_3)(\phi_1^+ \phi_1) + (\phi_3^+ \phi_2)(\phi_2^+ \phi_2) \right\} \\
&\quad + \lambda_7 \left\{ (\phi_1^+ \phi_1)(\phi_3^+ \phi_3) + (\phi_2^+ \phi_2)(\phi_3^+ \phi_3) + \text{h.c.} \right\} + \lambda_8(\phi_3^+ \phi_3)^2. \quad (3c)
\end{align}

In general $\lambda_4$ and $\lambda_7$ can be complex, but we assume them to be real so that CP symmetry is not broken explicitly. For the stability of the vacuum in the asymptotic limit we impose the requirement that there should be no direction in the field space along which the potential becomes infinitely negative. The necessary and sufficient conditions for this is well known in the context of two Higgs-doublet models (2HDMs) $[32]$. For the potential of Eq. (3), a 2HDM equivalent situation arise if one of the doublets is made identically zero. Then it is quite straightforward to find the following \textit{necessary} conditions for the global stability in the asymptotic limit:

\begin{align}
\lambda_1 &> 0, \quad (4a) \\
\lambda_8 &> 0, \quad (4b) \\
\lambda_1 + \lambda_3 &> 0, \quad (4c) \\
2\lambda_1 + (\lambda_3 - \lambda_2) &> |\lambda_2 + \lambda_3|, \quad (4d) \\
\lambda_5 + 2\sqrt{\lambda_8(\lambda_1 + \lambda_3)} &> 0, \quad (4e) \\
\lambda_5 + \lambda_6 + 2\sqrt{\lambda_8(\lambda_1 + \lambda_3)} &> 2|\lambda_7|, \quad (4f) \\
\lambda_1 + \lambda_3 + \lambda_5 + \lambda_6 + 2\lambda_7 + \lambda_8 &> 2|\lambda_4|. \quad (4g)
\end{align}

To avoid confusion, we wish to mention that an equivalent doublet representation,

\begin{align}
\begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad (5)
\end{align}

has also been used in the literature. In terms of this new doublet, the quartic part of the scalar potential is written as $[33-35]$:

\begin{align}
V_4 &= \frac{\beta_1}{2} \left( \chi_1^+ \chi_1 + \chi_2^+ \chi_2 \right)^2 + \frac{\beta_2}{2} \left( \chi_1^+ \chi_1 - \chi_2^+ \chi_2 \right)^2 + \beta_3(\chi_1^+ \chi_2)(\chi_2^+ \chi_1) + \frac{\beta_4}{2}(\phi_3^+ \phi_3)^2
\end{align}
\[ + \beta_5 (\phi_3^\dagger \phi_3)(\chi_1^\dagger \chi_1 + \chi_2^\dagger \chi_2) + \beta_6 \phi_3^\dagger (\chi_1 \chi_1^\dagger + \chi_2 \chi_2^\dagger) \phi_3 + \beta_7 \{ (\phi_3^\dagger \chi_1)(\phi_3^\dagger \chi_2) + \text{h.c.} \} \nonumber \\
+ \beta_8 \{ \phi_3^\dagger (\chi_1 \chi_2^\dagger \chi_1 + \chi_2 \chi_2^\dagger \chi_2) + \text{h.c.} \} . \] 

(6)

It is easy to verify that the parameters of Eq. (6) are related to the parameters of Eq. (3c) in the following way:

\[ \beta_1 = 2 \lambda_1 ; \quad \beta_2 = -2 \lambda_2 ; \quad \beta_3 = 4 \lambda_3 ; \quad \beta_4 = 2 \lambda_8 ; \quad \beta_5 = \lambda_5 ; \quad \beta_6 = \lambda_6 ; \quad \beta_7 = 2 \lambda_7 ; \quad \beta_8 = -\sqrt{2} \lambda_4 . \] 

(7)

This mapping can be used to translate the constraints on \( \lambda \)s into constraints on \( \beta \)s. In this paper we opt to work with the parametrization of Eq. (3).

### 3 Physical eigenstates

We represent the scalar doublets in the following way:

\[ \phi_k = \left( \begin{array}{c} w_k^+ \\
\frac{i}{\sqrt{2}} (v_k + h_k + iz_k) \end{array} \right) \quad \text{for} \quad k = 1, 2, 3. \] 

(8)

We shall assume that CP symmetry is not spontaneously broken and so the vacuum expectation values (vevs) are taken to be real. They also satisfy the usual vev relation: \( v = \sqrt{v_1^2 + v_2^2 + v_3^2} = 246 \text{ GeV} \). The minimization conditions for the scalar potential of Eq. (3) reads:

\[ \begin{align*}
\mu_1^2 &= -2 \lambda_1 (v_1^2 + v_2^2) - 2 \lambda_3 (v_1^2 + v_3^2) - v_3 \{ 6 \lambda_4 v_2 + (\lambda_5 + \lambda_6 + 2 \lambda_7) v_1 \} , \\
\mu_2^2 &= -2 \lambda_1 (v_1^2 + v_2^2) - 2 \lambda_3 (v_1^2 + v_3^2) - \frac{3 v_3}{v_2} 3 \lambda_4 (v_1^2 - v_2^2) - (\lambda_5 + \lambda_6 + 2 \lambda_7) v_3^2 , \\
\mu_3^2 &= \lambda_4 v_3^2 (v_2^2 - v_3^2) - (\lambda_5 + \lambda_6 + 2 \lambda_7) (v_1^2 + v_2^2) - 2 \lambda_8 v_3^2 . 
\end{align*} \] 

(9a, 9b, 9c)

For the self-consistency of Eqs. (9a) and (9b), two possible scenarios arise:

\[ \lambda_4 = 0 , \] 

or \( v_1 = \sqrt{3} v_2 . \) 

(10a, 10b)

In the following subsections we shall discuss each of the above scenarios separately.

#### 3.1 Case-I \( (\lambda_4 = 0) \)

Since CP symmetry is assumed to be exact in the scalar potential, the neutral physical states will be eigenstates of CP too. We find that the mass-squared matrices in the scalar\( (M_S^2) \), pseudoscalar\( (M_P^2) \) and charged\( (M_C^2) \) sectors are simultaneously block diagonalizable by the following matrix:

\[ X = \begin{pmatrix} \cos \gamma & -\sin \gamma & 0 \\
\sin \gamma & \cos \gamma & 0 \\
0 & 0 & 1 \end{pmatrix} \quad \text{with} \quad \tan \gamma = \frac{v_1}{v_2} . \] 

(11)

For the charged mass matrix, we obtain:

\[ X M_C^2 X^T = \begin{pmatrix} m_{1+}^2 & 0 & 0 \\
0 & -\frac{1}{2} v_3^2 (\lambda_6 + 2 \lambda_7) & \frac{1}{2} v_3 \sqrt{v_1^2 + v_2^2 \lambda_6 + 2 \lambda_7) \\
0 & \frac{1}{2} \sqrt{v_1^2 + v_2^2} (\lambda_6 + 2 \lambda_7) & -\frac{1}{2} (v_1^2 + v_2^2) (\lambda_6 + 2 \lambda_7) \end{pmatrix} , \] 

(12)

where, one of the charged Higgs \( (H_1^+) \) with mass \( m_{1+} \), is defined as:

\[ H_1^+ = \cos \gamma \ w_1^+ - \sin \gamma \ w_2^+ , \] 

(13a)

\footnote{Another possibility, \( v_3 = 0 \), while mathematically consistent, is unattractive. This is because, in some \( S_3 \) structure of the Yukawa sector, the \( S_3 \)-singlet fermion generation will the remain massless.}
Finally, for the CP-even part we have:

\[ m_{A_1}^2 = - \left\{ 2\lambda_3 \sin^2 \beta + \frac{1}{2}(\lambda_6 + 2\lambda_7) \cos^2 \beta \right\} v^2, \]  

with \[ \tan \beta = \frac{\sqrt{v_1^2 + v_2^2}}{v_3}. \]

The second charged Higgs \( H_2^+ \) along with the massless Goldstone \( (\omega^+) \), which will appear as the longitudinal component of the \( W \)-boson, can be obtained by diagonalizing the remaining \( 2 \times 2 \) block:

\[
\begin{pmatrix}
H_2^+ \\
\omega^+
\end{pmatrix} = \begin{pmatrix}
\cos \beta & -\sin \beta \\
\sin \beta & \cos \beta
\end{pmatrix}
\begin{pmatrix}
w_2^+ \\
w_3^+
\end{pmatrix}
\]

with \( w_2^+ = \sin \gamma w_1^+ + \cos \gamma w_2^+ \).

The mass of the second charged Higgs is given by:

\[ m_{A_1}^2 = -\frac{1}{2}(\lambda_6 + 2\lambda_7)v^2. \]

Similar considerations for the pseudoscalar part gives:

\[
XM_{A_1}^{P}X^T = \begin{pmatrix}
\frac{1}{2}m_{A_1}^2 & 0 & 0 \\
0 & -v_3^2 \lambda_7 & v_3(\sqrt{v_1^2 + v_2^2} \lambda_7) \\
0 & v_3(\sqrt{v_1^2 + v_2^2} \lambda_7) & -(v_1^2 + v_2^2) \lambda_7
\end{pmatrix},
\]

where, the pseudoscalar state \((A_1)\) with mass eigenvalue \( m_{A_1} \) is defined as:

\[
\begin{align*}
A_1 &= \cos \gamma z_1 - \sin \gamma z_2, \\
m_{A_1}^2 &= -2 \left\{ (\lambda_2 + \lambda_3) \sin^2 \beta + \lambda_7 \cos^2 \beta \right\} v^2,
\end{align*}
\]

where, \( \tan \beta \) has already been defined in Eq. (13c). Similar to the charged part, here also the second pseudoscalar \((A_2)\) along with the massless Goldstone \((\zeta)\) can be obtained as follows:

\[
\begin{pmatrix}
A_2 \\
\zeta
\end{pmatrix} = \begin{pmatrix}
\cos \beta & -\sin \beta \\
\sin \beta & \cos \beta
\end{pmatrix}
\begin{pmatrix}
z_2' \\
z_1'
\end{pmatrix}
\]

with \( z_2' = \sin \gamma z_1 + \cos \gamma z_2 \),

and, \[ m_{A_2}^2 = -2\lambda_7 v^2. \]

Finally, for the CP-even part we have:

\[
XM_{A_2}^{P}X^T = \begin{pmatrix}
0 & 0 & 0 \\
0 & A_S' & -B_S' \\
0 & -B_S' & C_S'
\end{pmatrix},
\]

where, \( A_S' = (\lambda_1 + \lambda_3)(v_1^2 + v_2^2) \),

\( B_S' = -\frac{1}{2}v_3 \sqrt{v_1^2 + v_2^2}(\lambda_5 + \lambda_6 + 2\lambda_7) \),

\( C_S' = \lambda_8 v_3^2 \).

The massless state \((h^0)\), as also noted in [36], is given by:

\[ h^0 = \cos \gamma h_1 - \sin \gamma h_2. \]

But we wish to add here that the appearance of a massless scalar is not surprising. One can easily verify that the potential of Eq. (3) has the following \( SO(2) \) symmetry for \( \lambda_4 = 0 \):

\[
\begin{pmatrix}
\phi_1' \\
\phi_2'
\end{pmatrix} = \begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix}
\begin{pmatrix}
\phi_1 \\
\phi_2
\end{pmatrix}
\]

Since \( SO(2) \) is a continuous symmetry isomorphic to \( U(1) \), a massless physical state is expected. Other two physical scalars are obtained as follows:

\[
\begin{pmatrix}
h \\
H
\end{pmatrix} = \begin{pmatrix}
\cos \alpha & -\sin \alpha \\
\sin \alpha & \cos \alpha
\end{pmatrix}
\begin{pmatrix}
h_2' \\
h_3'
\end{pmatrix}
\]

with \( h_2' = \sin \gamma h_1 + \cos \gamma h_2 \),
and,  \[ \tan 2\alpha = \frac{2B'S}{A'S - C'S}. \]  

(22b)

We assume \( H \) and \( h \) to be the heavier and lighter CP-even mass eigenstates respectively, with the following eigenvalues:

\[
m^2_H = (A'S + C'S) + \sqrt{(A'S - C'S)^2 + 4B'^2S},
\]

(23a)

\[
m^2_h = (A'S + C'S) - \sqrt{(A'S - C'S)^2 + 4B'^2S}.
\]

(23b)

At this stage, it is worth noting that we can define two intermediate scalar states, \( H^0 \) and \( R \), as

\[
\begin{pmatrix} R \\ H^0 \end{pmatrix} = \begin{pmatrix} \cos \beta & -\sin \beta \\ \sin \beta & \cos \beta \end{pmatrix} \begin{pmatrix} h'_2 \\ h_3 \end{pmatrix},
\]

(24)

with the property that \( H^0 \) has the exact SM couplings with the vector boson pairs and fermions. \( H^0 \) does not take part in the flavor changing processes as well. Of course, \( H^0 \) and \( R \) are not the physical eigenstates in general but are related to them in the following way:

\[
\begin{align*}
 h &= \cos(\beta - \alpha)R + \sin(\beta - \alpha)H^0, \\
 H &= -\sin(\beta - \alpha)R + \cos(\beta - \alpha)H^0.
\end{align*}
\]

(25a)

(25b)

In view of the fact that a 125 GeV scalar with SM-like properties has already been observed at the LHC, we wish the lighter CP-even mass eigenstate \( (h) \) to coincide with \( H^0 \). Then we must require:

\[ \cos(\beta - \alpha) \approx 0. \]

(26)

In analogy with the 2HDM case \cite{32}, this limit can be taken as the \textit{decoupling limit} in the context of a 3HDM with an \( S_3 \) symmetry. We must emphasize though, the term ‘decoupling limit’ does not necessarily imply the heaviness of the additional scalars. Considering Eqs. (20) and (24), it is also interesting to note that the state \( h^0 \), being orthogonal to \( H^0 \), does not have any trilinear \( h^0VV \) (\( V = W, Z \)) coupling. But, in general, it will have flavor changing coupling in the Yukawa sector. This type of neutral massless state with flavor changing fermionic coupling will be ruled out from the well measured values of neutral meson mass differences. This means that the choice \( \lambda_4 = 0 \) is phenomenologically unacceptable and we shall not pursue this scenario any further.

### 3.2 Case-II \((v_1 = \sqrt{3}v_2)\)

This situation has recently been analyzed in \cite{37}. We, however, use a convenient parametrization that can provide intuitive insight into the scenario and additionally, we also discuss the possibility of a \textit{decoupling limit} in the same way as done in the previous subsection.

The definitions for the angles, \( \gamma \) and \( \beta \), and the diagonalizing matrix, \( X \), remain the same as before. Only difference is that, due to the vev alignment \((v_1 = \sqrt{3}v_2)\), \( \tan \gamma (= \sqrt{3}) \) and hence \( X \) is determined completely. Now only two of the vevs, \( v_2 \) and \( v_3 \) (say), can be considered independent and \( \tan \beta \) is given in terms of them as follows:

\[ \tan \beta = \frac{2v_2}{v_3}. \]

(27)

The charged and pseudoscalar mass eigenstates have the same form as before; only the mass eigenvalues get modified due to the presence of \( \lambda_4 \):

\[
m^2_{1+} = -\left\{ 2\lambda_3 \sin^2 \beta + \frac{5}{2} \lambda_4 \sin \beta \cos \beta + \frac{1}{2}(\lambda_6 + 2\lambda_7) \cos^2 \beta \right\} v^2,
\]

(28a)

\[
m^2_{2+} = -\frac{1}{2} \{ \lambda_4 \tan \beta + (\lambda_6 + 2\lambda_7) \} v^2,
\]

(28b)
\[ m_{A_1}^2 = - \left\{ 2(\lambda_2 + \lambda_3) \sin^2 \beta + \frac{5}{2} \lambda_4 \sin \beta \cos \beta + 2 \lambda_7 \cos^2 \beta \right\} v^2 , \]  
\[ m_{A_2}^2 = - \left( \frac{1}{2} \lambda_4 \tan \beta + 2 \lambda_7 \right) v^2 . \]  
(28c)
(28d)

In the presence of \( \lambda_4 \), analysis of the scalar part will be slightly different:

\[
XM_S^2 X^T = \begin{pmatrix} \frac{1}{2} m_{h_0}^2 & 0 & 0 \\ 0 & A_S & -B_S \\ 0 & -B_S & C_S \end{pmatrix} ,
\]

where, \( A_S = (\lambda_2 + \lambda_3) v^2 \sin^2 \beta + \frac{3}{4} \lambda_4 v^2 \sin \beta \cos \beta , \)
(29a)
(29b)
(29c)
(29d)

\[
B_S = -\frac{1}{2} \left\{ \frac{3}{2} \lambda_4 \sin^2 \beta + (\lambda_5 + \lambda_6 + 2 \lambda_7) \sin \beta \cos \beta \right\} v^2 , \]

\[
C_S = -\frac{\lambda_4}{4} v^2 \sin^2 \beta \tan \beta + \lambda_8 v^2 \cos^2 \beta . \]

The state, \( h^0 \), will no longer be massless, in fact,

\[
m_{h_0}^2 = - \frac{9}{2} \lambda_4 v^2 \sin \beta \cos \beta . \]  
(30)

The angle \( \alpha \), which was used to rotate from \((h_2^*, h_3)\) basis to the physical \((H, h)\) basis, should be redefined as:

\[
\tan 2\alpha = \frac{2B_S}{A_S - C_S} , \]  
(31)

and corresponding mass eigenvalues should have the following expressions:

\[
m_H^2 = (A_S + C_S) + \sqrt{(A_S - C_S)^2 + 4B_S^2} , \]  
(32a)
\[
m_h^2 = (A_S + C_S) - \sqrt{(A_S - C_S)^2 + 4B_S^2} . \]  
(32b)

The conclusion of the previous subsection that in the decoupling limit, \( \cos(\beta - \alpha) = 0 \), \( h \) possesses SM-like gauge and Yukawa couplings, still holds. It should be emphasized that the Yukawa couplings of \( h \) in this limit, resembles that of the SM, do not depend on the transformation properties of the fermions under \( S_3 \).

Also, the self couplings of \( h \) coincides with the corresponding SM expressions in the decoupling limit:

\[
\mathcal{L}_{\text{h eff}}^\text{sm} = -\frac{m_H^2}{2v} h^3 - \frac{m_h^2}{8v^2} h^4 . \]  
(33)

Similar to the case described in the previous subsection, \( h^0 \) will not have any \( h^0VV \) \((V = W, Z)\) couplings, but in the present scenario, we may identify a symmetry which forbids such couplings. Note that, when the specified relation between \( v_1 \) and \( v_2 \) is taken, there exists a two dimensional representation of \( \mathbb{Z}_2 \):

\[
\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \frac{1}{2} \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} , \]
(34)

which was initially a subgroup of the original \( S_3 \) symmetry, remains intact even after the spontaneous symmetry breaking, i.e., the vacuum is invariant under this \( \mathbb{Z}_2 \) symmetry. This allows us to assign a \( \mathbb{Z}_2 \) parity for different physical states and this should be conserved in the theory. The state \( h^0 \) is odd under this \( \mathbb{Z}_2 \) and this is what forbids it to couple with the \( V \) pair. In fact, using the assignments of Table 1, together with CP symmetry, many of the scalar self couplings can be inferred to be zero.

In connection with the number of independent parameters in the Higgs potential, we note that there were ten to start with \((\mu_{1, 3} \text{ and } \lambda_{1, 2, \ldots, 8})\). \( \mu_1 \) and \( \mu_3 \) can be traded for \( v_1 \) and \( v_3 \) or, equivalently for \( v \) and
 supersymmetry. The remaining eight $\lambda$s can be traded for seven physical Higgs masses and $\alpha$. The connections are given below:

$$
\begin{align*}
\lambda_1 &= \frac{1}{2v^2 \sin^2 \beta} \left\{ \left( m_h^2 \cos^2 \alpha + m_H^2 \sin^2 \alpha \right) + \left( m_{1+}^2 - m_{2+}^2 \cos^2 \beta - \frac{1}{9} m_{h0}^2 \right) \right\}, \\
\lambda_2 &= \frac{1}{2v^2 \sin^2 \beta} \left\{ \left( m_{1+}^2 - m_{A1}^2 \right) - \left( m_{2+}^2 - m_{A2}^2 \right) \cos^2 \beta \right\}, \\
\lambda_3 &= \frac{1}{2v^2 \sin^2 \beta} \left( \frac{4}{9} m_{h0}^2 + m_{2+}^2 \cos^2 \beta - m_{1+}^2 \right), \\
\lambda_4 &= \frac{2}{9} m_{h0}^2 + \frac{1}{v^2} \sin \beta \cos \beta, \\
\lambda_5 &= \frac{1}{v^2} \left\{ \sin \frac{\alpha \cos \alpha}{\sin \beta \cos \beta} \left( m_H^2 - m_h^2 \right) + 2m_{2+}^2 + \frac{1}{9} m_{h0}^2 \right\}, \\
\lambda_6 &= \frac{1}{v^2} \left( \frac{1}{9} m_{h0}^2 \cos^2 \beta + m_{A2}^2 - 2m_{2+}^2 \right), \\
\lambda_7 &= \frac{1}{v^2} \left( \frac{1}{9} m_{h0}^2 \cos^2 \beta - m_{A2}^2 \right), \\
\lambda_8 &= \frac{1}{2v^2 \cos^2 \beta} \left\{ \left( m_h^2 \sin^2 \alpha + m_H^2 \cos^2 \alpha \right) - \frac{1}{9} m_{h0}^2 \tan^2 \beta \right\}.
\end{align*}
$$

In passing, we wish to state that for the analysis purpose we will always be working in the decoupling limit with $v_1 = \sqrt{3}v_2$.

4 Constraints from unitarity

In this context, the pioneering work has been done by Lee, Quigg and Thacker (LQT) [26]. They have analyzed several two body scatterings involving longitudinal gauge bosons and physical Higgs in the SM. All such scattering amplitudes are proportional to Higgs quartic coupling in the high energy limit. The $\ell = 0$ partial wave amplitude ($a_0$) is then extracted from these amplitudes and cast in the form of an S-matrix having different two-body states as rows and columns. The largest eigenvalue of this matrix is bounded by the unitarity constraint, $|a_0| < 1$. This restricts the quartic Higgs self coupling and therefore the Higgs mass to a maximum value.

The procedure has been extended to the case of a 2HDM scalar potential [38–41]. We take it one step further and apply it in the context of 3HDMs. Here also same types of two body scattering channels are considered. Thanks to the equivalence theorem [42, 43], we can use unphysical Higgses instead of actual longitudinal components of the gauge bosons when considering the high energy limit. So, we can use the Goldstone-Higgs potential of Eq. (3) for this analysis. Still it will be a much involved calculation. But we notice that the diagrams containing trilinear vertices will be suppressed by a factor of $E^2$ coming from the intermediate propagator. Thus they do not contribute at high energies, only the quartic couplings contribute. Clearly the physical Higgs masses that could come from the propagators, do not enter this analysis. Since we are interested only in the eigenvalues of the S-matrix, this allows us to work with the original fields of Eq. (3c) instead of the physical mass eigenstates. After an inspection of all the neutral and charged two-body channels, we find the following eigenvalues to be bounded from unitarity:

$$
|a_i^0|, |b_i| \leq 16\pi, \text{ for } i = 1, 2, \ldots, 6.
$$

| Physical States | Transformation under $Z_2$ |
|-----------------|-----------------------------|
| $h^0, H_1^\pm, A_1$ | Odd |
| $H^0, R, H_2^\pm, A_2$ | Even |

Table 1: $Z_2$ parity assignments to the physical mass eigenstates.
Figure 1: (Case-II) Regions allowed from unitarity and stability. We have fixed $m_h$ at 125 GeV and taken $m_{1+}, m_{2+} > 80$ GeV and $m_{H}, m_{h0} > m_h$.

The expressions for the individual eigenvalues in terms of $\lambda$s are given below:

\begin{align*}
a_1^\pm &= \left( \lambda_1 - \lambda_2 + \frac{\lambda_5 + \lambda_6}{2} \right) \pm \sqrt{\left( \lambda_1 - \lambda_2 + \frac{\lambda_5 + \lambda_6}{2} \right)^2 - 4 \left( (\lambda_1 - \lambda_2) \left( \frac{\lambda_5 + \lambda_6}{2} \right) - \lambda_3^2 \right)}, \quad (37a) \\
a_2^\pm &= (\lambda_1 + \lambda_2 + 2\lambda_3 + \lambda_8) \pm \sqrt{(\lambda_1 + \lambda_2 + 2\lambda_3 + \lambda_8)^2 - 4 \left( \lambda_8 (\lambda_1 + \lambda_2 + 2\lambda_3) - 2\lambda_2^2 \right)}, \quad (37b) \\
a_3^\pm &= (\lambda_1 - \lambda_2 + 2\lambda_3 + \lambda_8) \pm \sqrt{(\lambda_1 - \lambda_2 + 2\lambda_3 + \lambda_8)^2 - 4 \left( \lambda_8 (\lambda_1 - \lambda_2 + 2\lambda_3) - \frac{\lambda_2^2}{2} \right)}, \quad (37c) \\
a_4^\pm &= \left( \lambda_1 + \lambda_2 + \frac{\lambda_5}{2} + \lambda_7 \right) \pm \sqrt{\left( \lambda_1 + \lambda_2 + \frac{\lambda_5}{2} + \lambda_7 \right)^2 - 4 \left( (\lambda_1 + \lambda_2) \left( \frac{\lambda_5}{2} + \lambda_7 \right) - \lambda_3^2 \right)}, \quad (37d) \\
a_5^\pm &= (5\lambda_1 - \lambda_2 + 2\lambda_3 + 3\lambda_8) \\
&\quad \pm \sqrt{(5\lambda_1 - \lambda_2 + 2\lambda_3 + 3\lambda_8)^2 - 4 \left( 3\lambda_8 (5\lambda_1 - \lambda_2 + 2\lambda_3) - \frac{1}{2} (2\lambda_5 + \lambda_6)^2 \right)}, \quad (37e) \\
a_6^\pm &= \left( \lambda_1 + \lambda_2 + 4\lambda_3 + \frac{\lambda_5}{2} + \lambda_6 + 3\lambda_7 \right) \\
&\quad \pm \sqrt{(\lambda_1 + \lambda_2 + 4\lambda_3 + \frac{\lambda_5}{2} + \lambda_6 + 3\lambda_7)^2 - 4 \left( (\lambda_1 + \lambda_2 + 4\lambda_3) \left( \frac{\lambda_5}{2} + \lambda_6 + 3\lambda_7 \right) - 9\lambda_3^2 \right)}, \quad (37f) \\
b_1 &= \lambda_5 + 2\lambda_6 - 6\lambda_7, \quad (37g) \\
b_2 &= \lambda_5 - 2\lambda_7, \quad (37h) \\
b_3 &= 2(\lambda_1 - 5\lambda_2 - 2\lambda_3), \quad (37i)
\end{align*}
Figure 2: Signal strengths for diphoton and Z-photon decay modes within the allowed range for charged Higgs masses.

\[
b_4 = 2(\lambda_1 - \lambda_2 - 2\lambda_3), \quad \text{(37j)}
\]
\[
b_5 = 2(\lambda_1 + \lambda_2 - 2\lambda_3), \quad \text{(37k)}
\]
\[
b_6 = \lambda_5 - \lambda_6. \quad \text{(37l)}
\]

In passing, we remark that the perturbativity criteria, \(|\lambda_i| < 4\pi\), coming from the requirement that the leading order contribution to the physical amplitude must have higher magnitude than the subleading order, may have some ambiguity in this context. This is due to the fact the individual \(\lambda_i\) do not appear in the quartic couplings involving the physical scalars. Hence the combination of \(\lambda_i\), that constitute the physical couplings, should be used for this purpose and it does not necessarily imply that the individual \(\lambda_i\) should be bounded. We have presented here the exact constraints on \(\lambda_i\) which should be satisfied for unitarity not to be violated.

Eqs. (4) and (37) can be used to put limits on the physical Higgs masses. For this purpose, we work in the decoupling limit taking the lightest scalar \((h)\) to be the SM-like Higgs that has been found at the LHC and we set its mass at 125 GeV. We also assume the charged scalars \( (m_{1+} \text{ and } m_{2+})\) to be heavier than 80 GeV to respect the direct search bound from LEP2 [44]. To collect sufficient number of data points we have generated fifty million random sets of \{\(\tan \beta, m_{h0}, m_H, m_{A1}, m_{A2}, m_{1+}, m_{2+}\}\) by varying \(\tan \beta\) from 0.1 to 100 and filter them through the combined constraints from unitarity and stability. The sets that survive the filtering are plotted in Figure 1. The bounds that follow from these figures are listed below:

- \(\tan \beta \in [0.3, 17],\)
- \(m_{h0} < 870 \text{ GeV}, m_H < 880 \text{ GeV}, m_{A1} < 940 \text{ GeV}, m_{A2} < 910 \text{ GeV}, m_{1+} < 940, m_{2+} < 910 \text{ GeV}.\)

It is interesting to note that, if the observed scalar at the LHC has its root in the S3HDM, then there must be several other nonstandard scalars with masses below 1 TeV.

5 Impact on loop induced Higgs decays

As already has been pointed out, in the decoupling limit the lightest scalar \((h)\) couples with fermions and gauge bosons exactly in the SM way. Consequently, the production cross section as well as tree level decay branching ratios will not alter from their respective SM values. However, the loop induced decay modes like, \(h \to \gamma \gamma\) and \(h \to Z \gamma\), will pick up additional contributions due to the presence of nonstandard charged scalar loops. Note that the change in total Higgs decay width will be negligibly small as the branching fractions of such decays are tiny.
To display the contribution of the charged scalar loops to the decay amplitudes in a convenient form, we define dimensionless parameters, $\kappa_i$ ($i = 1, 2$), in the following way:

$$
g_{hH^+H^-} = \kappa_i \frac{g m_i^2}{M_W}.
$$

The standard expression for the diphoton decay width is given by [45]:

$$
\Gamma(h \rightarrow \gamma \gamma) = \frac{\alpha^2 g^2}{2^{10} \pi^3} \frac{m_h^3}{M_W^2} \left| \mathcal{F}_W + \frac{4}{3} \mathcal{F}_t + \sum_{i=1}^2 \kappa_i \mathcal{F}_{i+} \right|^2,
$$

where, using the notation $\tau_x \equiv (2m_x/m_h)^2$, the expressions for $\mathcal{F}_W$, $\mathcal{F}_t$ and $\mathcal{F}_{i+}$ ($i = 1, 2$) are given by,

$$
\begin{align*}
\mathcal{F}_W & = 2 + 3\tau_W + 3\tau_W(2-\tau_W) f(\tau_W), \quad (40a) \\
\mathcal{F}_t & = -2\tau_t \left[ 1 + (1 - \tau_t) f(\tau_t) \right], \quad (40b) \\
\mathcal{F}_{i+} & = -\tau_{i+} \left[ 1 - \tau_{i+} f(\tau_{i+}) \right]. \quad (40c)
\end{align*}
$$

For the values of masses that we are dealing with, makes $\tau_x > 1$ for $x = W, t, H^+_i$ and then

$$
f(\tau) = \left[ \sin^{-1} \left( \sqrt{1/\tau} \right) \right]^2.
$$

The decay width for $h \rightarrow Z \gamma$ is given by:

$$
\Gamma(h \rightarrow Z \gamma) = \frac{\alpha^2 g^2}{2^9 \pi^3} \frac{m_h^3}{M_W^2} \left| \mathcal{A}_W + \mathcal{A}_t + \sum_{i=1}^2 \kappa_i \mathcal{A}_{i+} \right|^2 \left( 1 - \frac{M_Z^2}{m_h^2} \right)^3,
$$

where, using $\eta_x = (2m_x/M_Z)^2$, the expressions for $\mathcal{A}_W$, $\mathcal{A}_t$ and $\mathcal{A}_{i+}$ are given by [45],

$$
\begin{align*}
\mathcal{A}_W & = \cot \theta_w \left[ 4(\tan^2 \theta_w - 3) I_2(\tau_W, \eta_W) \\
& \quad + \left\{ \left( 5 + \frac{2}{\tau_W} \right) - \left( 1 + \frac{2}{\tau_W} \right) \tan^2 \theta_w \right\} I_1(\tau_W, \eta_W) \right], \quad (43a) \\
\mathcal{A}_t & = \frac{4(\frac{1}{2} - \frac{3}{2} \sin^2 \theta_w)}{\sin \theta_w \cos \theta_w} \left[ I_2(\tau_t, \eta_t) - I_1(\tau_t, \eta_t) \right], \quad (43b) \\
\mathcal{A}_{i+} & = \frac{2\sin^2 \theta_w - 1}{\sin \theta_w \cos \theta_w} I_1(\tau_{i+}, \eta_{i+}). \quad (43c)
\end{align*}
$$

The functions $I_1$ and $I_2$ are defined as,

$$
\begin{align*}
I_1(\tau, \eta) & = \frac{\tau \eta}{2(\tau - \eta)} + \frac{\tau^2 \eta^2}{2(\tau - \eta)^2} \left[ f(\tau) - f(\eta) \right] + \frac{\tau^2 \eta}{(\tau - \eta)^2} \left[ g(\tau) - g(\eta) \right], \quad (44a) \\
I_2(\tau, \eta) & = -\frac{\tau \eta}{2(\tau - \eta)} \left[ f(\tau) - f(\eta) \right], \quad (44b)
\end{align*}
$$

where the function $f$ has the same definition as in Eq. (41). Since $\tau_x, \eta_x > 1$ for $x = W, t, H^+_i$, the function $g$ takes the following form:

$$
g(x) = \sqrt{x - 1} \sin^{-1} \left( \sqrt{1/x} \right). \quad (45)
$$

In the decoupling limit, the parameters $\kappa_i$ ($i = 1, 2$), which appear in Eqs. (38), (39) and (42) are given by,

$$
\kappa_i = - \left( 1 + \frac{m_i^2}{2m_{i+}^2} \right). \quad (46)
$$
In our case, the signal strengths $\mu_{\gamma\gamma}$ and $\mu_{Z\gamma}$, defined through the equations,

$$
\mu_{\gamma\gamma} = \frac{\sigma(pp \to h)}{\sigma^{SM}(pp \to h)} \cdot \frac{\text{BR}(h \to \gamma\gamma)}{\text{BR}^{SM}(h \to \gamma\gamma)},
$$

$$
\mu_{Z\gamma} = \frac{\sigma(pp \to h)}{\sigma^{SM}(pp \to h)} \cdot \frac{\text{BR}(h \to Z\gamma)}{\text{BR}^{SM}(h \to Z\gamma)},
$$

(47)

(48)

assume the following forms:

$$
\mu_{\gamma\gamma} = \frac{\Gamma(h \to \gamma\gamma)}{\Gamma^{SM}(h \to \gamma\gamma)} = \left| \mathcal{F}_W + \frac{4}{3} \mathcal{F}_t + \sum_{i=1}^{2} \kappa_i \mathcal{F}_{i+} \right|^2 \left| \mathcal{F}_W + \frac{4}{3} \mathcal{F}_t \right|^2,
$$

(49)

$$
\mu_{Z\gamma} = \frac{\Gamma(h \to Z\gamma)}{\Gamma^{SM}(h \to Z\gamma)} = \left| A_W + A_t + \sum_{i=1}^{2} \kappa_i A_{i+} \right|^2 \left| A_W + A_t \right|^2.
$$

(50)

As the charged Higgs becomes heavy, the quantity $\mathcal{F}_{i+}$, for example, saturates to $\frac{1}{3}$. So the decoupling of charged Higgs from loop induced Higgs decay depends on how $\kappa_i$ behaves with increasing $m_{i+}$. It follows from Eq. (46) that $\kappa_i \to -1$ if $m_{i+} \gg m_h$. Consequently, the charged Higgs never decouples from the diphoton or $Z$-photon decay amplitudes. In fact, it reduces the decay widths from their corresponding SM expectations. These features have been displayed in Figure 2 where we have made a contour plot by varying the charged Higgs masses within the allowed ranges coming from unitarity and vacuum stability. We find that $\mu_{\gamma\gamma}$ and $\mu_{Z\gamma}$ should lie within $[0.42, 0.80]$ and $[0.73, 0.93]$ for $m_{1+} \in [80, 950]$ and $m_{2+} \in [80, 950]$. We must admit though, this nondecoupling of charged scalar is not a unique feature of a S3HDM as it is also known to be present in the context of a 2HDMs [46–49]. Currently the ATLAS data favor an enhancement whereas the data from CMS favor a suppression in the diphoton decay channel [50]. Thus a precise measurement of the diphoton and Z-photon signal strengths can pin down the difference between the SM Higgs and a SM-like Higgs arising from an extended scalar sector.

6 Conclusions

In this article we have analyzed in detail the scalar sector of an S3HDM. Our findings are listed below:

- The minimization of the scalar potential leads to a specific relation between the vevs of the first two doublets, $v_1 = \sqrt{3} v_2$ in particular.

- In this limit we find a $Z_2$ subgroup of $S_3$ that remains unbroken even after the spontaneous symmetry breaking. The different scalar mass eigenstates can then be assigned with appropriate $Z_2$ parity which can help us understand why certain couplings do not appear in the theory.

- Additionally, we have identified a decoupling limit for this model where the lightest CP-even scalar has the exact same coupling as the SM Higgs with the other SM particles.

- We have also derived the exact tree unitarity constraints and exploited them, in the decoupling limit, to put new bounds on the physical nonstandard Higgs masses, which we consider to be an important development in the multi-Higgs context.

- From unitarity and stability $\tan \beta$ is likely to be in the range $[0.3, 17]$ and all the nonstandard Higgs masses lie below 1 TeV.

- Regarding the decay of the SM-like $S_3$ Higgs, we have observed that the charged Higgs never decouples from the diphoton or $Z$-photon decay modes. The additional contributions from the charged Higgs loops to the decay amplitudes actually reduces the signal strengths of these modes. Although this depletion may not be a unique property of this scenario, but any statistically significant enhancement in $h \to \gamma\gamma$ and $h \to Z\gamma$ modes will certainly disfavor the possibility of an SM-like Higgs arising from an S3HDM.
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A Finding the unitarity constraints

In this appendix we present a detailed account of our discussions regarding unitarity bounds in Section 4. Any scattering amplitude can be expanded in terms of the partial waves as follows:

\[
\mathcal{M}(\theta) = 16\pi \sum_{\ell=0}^{\infty} a_\ell (2\ell + 1) P_\ell(\cos \theta),
\]  

where, \(\theta\) is the scattering angle and \(P_\ell(x)\) is the Legendre polynomial of order \(\ell\). The prescription is simple: once we calculate the Feynman amplitude of a certain \(2 \rightarrow 2\) scattering process, each of the partial wave amplitude \((a_\ell)\), in Eq. (51), can be extracted by using the orthonormality of the Legendre polynomials. As argued in Section 4, only the dimensionless quartic couplings will contribute to the amplitudes under consideration at high energies. For this, only \(\ell = 0\) partial amplitude \((a_0)\) will receive nonzero contribution from the leading order term in the scattering amplitude. It is our purpose, then, to find the expressions of \(a_0\) for every possible \(2 \rightarrow 2\) scattering process and cast them in the form of an S-matrix which is constructed by taking the different two-body channels as rows and columns. Unitarity will restrict the magnitude of each of the eigenvalues of this S-matrix to lie below unity. The resultant constraints have been in quoted in Eq. (37).

First important part of the calculation is to identify all the possible two-particle channels. These two-particle states are made of the fields \(w_i^\pm, h_i\) and \(z_k\) corresponding to the parametrization of Eq. (8). For our calculation, we consider neutral two-particle states \((e.g., w_i^+ w_j^-, h_i h_j, z_i z_j, h_i z_j)\) and singly charged two-particle states \((e.g., w_i^+ h_j, w_i^+ z_j)\). In general, if we have \(n\)-number of doublets \(\phi_k\) \((k = 1, \ldots, n)\) there will be \((3n^2 + n)\)-number of neutral and \(2n^2\)-number of charged two-particle states. Clearly, the dimensions of S-matrices formed out of these two-particle states will be a \((3n^2 + n) \times (3n^2 + n)\) and \(2n^2 \times 2n^2\) for the neutral and charged cases respectively. The eigenvalues of these matrices should be bounded by the unitarity constraint.

A.1 Neutral Channels:

In our case of three Higgs doublets there will be, \(3 \cdot (3)^2 + 3 = 30\) neutral two-particle states and thus the neutral channel S-matrix will be a \(30 \times 30\) matrix. The symmetries present in our potential, Eq. (3) and a few tricks allows us to get analytical expressions for the eigenvalues of this matrix. The basis of neutral two-particle states (NTPS) are,

\[
\{w_1^+ w_2, w_1^+ w_3, w_2^+ w_1^- w_1^-, w_3^+ w_1^- h_1 h_2, h_1 h_3, z_1 z_2, z_1 z_3, h_1 z_2, h_1 h_3, z_1 h_2, z_1 h_3\} \text{ and } \{h_3 z_3, h_1 z_1, h_2 z_2, h_3 z_2, h_2 z_3, h_3 z_3, w_1^+ w_2^-, w_1^+ w_3^- h_2 h_3, z_1 z_1, z_2 z_2, z_3 z_3\}
\]

Note that, the states containing two identical bosons contain an additional factor of \(1/\sqrt{2}\) due to boson symmetry. We divide the NTPS in two classes. This classification helps us to reduce, as a first level of simplification, the \(30 \times 30\) matrix to a \(12 \times 12\) and \(18 \times 18\) block diagonal form. If a bigger matrix can be block diagonalized in smaller matrices then the calculation of the eigenvalues of the original matrix becomes easier. In the present case this type of block diagonalization is possible due to the very structure of the potential. From the potential, Eq. (3) it is evident that transition from two-particle states containing even number of the index ‘1’ into two-particle states having odd number of ‘1’ and vice versa, are not allowed. This explains why the first set of NTPS above, are completely disentangled from the second set. The \(12 \times 12\) matrix constructed using the first set of NTPS is given by,

\[
\mathcal{M}^{(1)}_{NC} = \begin{pmatrix}
\mathcal{A}_{6 \times 6} & \mathcal{B}_{6 \times 6} \\
\mathcal{B}^\dagger_{6 \times 6} & \mathcal{C}_{6 \times 6}
\end{pmatrix},
\]

(52)
One can get analytical expressions of the eigenvalues of $\mathcal{M}_{\text{NC}}^{(1)}$ using MATHEMATICA. With reference to Eq. (37), these are $b_i$ ($i = 1, \ldots, 4$), $a^+_{ij}$ ($i = 1, 4, 6$) with $a^+_{ij}$ being twofold degenerate.

Now, the $18 \times 18$ matrix constructed using the second set of NTPS is $\mathcal{M}_{\text{NC}}^{(2)}$. To decompose it further into block diagonal form, we make use of the CP symmetry. Note that, $w^+_2 w^-_3$ and $w^-_2 w^+_3$ do not possess any definite CP properties but the linear combinations of them

$$w^-_{23} = \frac{1}{\sqrt{2}} (-w^+_2 w^-_3 + w^+_3 w^-_2), \quad \text{and}$$

$$w^+_{23} = \frac{1}{\sqrt{2}} (w^+_2 w^-_3 + w^+_3 w^-_2),$$

are CP-odd and CP-even states respectively. A closer look at the second set of NTPS reveals that the first five states are CP-odd whereas the last eleven states are CP-even. Clearly, if CP is conserved in the Higgs potential, then we may rotate the sixth and seventh states into $w^-_{23}$ and $w^+_{23}$ to assure the block diagonalization. Evidently the matrix, $U$, needed to perform unitary transformation on the original $18 \times 18$ matrix, can be constructed as follows:

$$U = \text{Block-diag}[X, Y, Z],$$

where,

$$X = \mathbf{1}_{5 \times 5}, \quad Y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad Z = \mathbf{1}_{11 \times 11}.$$
After the unitary transformation, we obtain the new matrix in the block diagonal form as given below,

$$\mathcal{M}^{(2)}_{NC} = U \mathcal{M}^{(2)}_{NC} U^\dagger = \begin{pmatrix} \mathcal{D}_{6\times6} & \mathcal{0}_{6\times12} \\ \mathcal{E}_{12\times6} & \mathcal{E}_{12\times12} \end{pmatrix},$$

(57)

where,

$$\mathcal{D} = \begin{pmatrix}
    h_{z3} & h_{2z3} & h_{3z2} & h_{z23} & h_{z23} & w_{z3} \\
    2\lambda_8 & 2\lambda_7 & 2\lambda_7 & 0 & 0 & 0 \\
    2\lambda_7 & 2(\lambda_1 + \lambda_3) & 2(\lambda_2 + \lambda_3) & \lambda_4 & \lambda_4 & 0 \\
    2\lambda_7 & 2(\lambda_2 + \lambda_3) & 2(\lambda_1 + \lambda_3) & -\lambda_4 & -\lambda_4 & 0 \\
    0 & \lambda_4 & -\lambda_4 & 2\lambda_7 & 2(\lambda_1 + \lambda_6 - 2\lambda_7) & \frac{i}{\sqrt{2}}(\lambda_6 - 2\lambda_7) \\
    0 & \lambda_4 & -\lambda_4 & 2\lambda_7 & \lambda_5 + \lambda_6 - 2\lambda_7 & \frac{i}{\sqrt{2}}(\lambda_6 - 2\lambda_7) \\
    w_{z3} & w_{z3} & w_{z3} & w_{z3} & w_{z3} & w_{z3} \\
    0 & 0 & 0 & \frac{i}{2}(\lambda_6 - 2\lambda_7) & \frac{i}{\sqrt{2}}(\lambda_6 - 2\lambda_7) & \lambda_5 + \lambda_6 - 4\lambda_7 \\
    0 & 0 & 0 & \sqrt{2}(\lambda_6 - 2\lambda_7) & \frac{i}{\sqrt{2}}(\lambda_6 - 2\lambda_7) & \lambda_5 + \lambda_6 - 4\lambda_7 \\
\end{pmatrix},$$

(58)

contains the CP-odd states and has eigenvalues $a_i^\pm$, $b_i$ for $i = 1, 2$ which are listed in Eq. (37). The matrix $\mathcal{H}$ can be written as,

$$\mathcal{E} = \begin{pmatrix} \mathcal{F}_{6\times6} & \mathcal{G}^T_{6\times6} \\ \mathcal{G}_{6\times6} & \mathcal{H}_{6\times6} \end{pmatrix},$$

(59)

where $\mathcal{F}$, $\mathcal{G}$ and $\mathcal{H}$ are given by,

$$\mathcal{F} = \begin{pmatrix}
    w_{z3} & h_{2z3} & z_{2z3} & w_{z3}^* w_{z3}^* & w_{z3}^* w_{z3}^* \frac{\lambda_5 + \lambda_6 + 4\lambda_7}{\sqrt{2}} \frac{\lambda_5 + \lambda_6 + 2\lambda_7}{\sqrt{2}} \\
    h_{2z3} & \lambda_5 + \lambda_6 + 2\lambda_7 & \frac{\lambda_5 + \lambda_6 + 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
    z_{2z3} & 2\lambda_7 & \frac{\lambda_5 + \lambda_6 + 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
    w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* \\
    w_{z3}^* & \frac{\lambda_5 + \lambda_6 + 4\lambda_7}{\sqrt{2}} & \frac{\lambda_5 + \lambda_6 + 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
\end{pmatrix},$$

$$\mathcal{G}^T = \begin{pmatrix}
    w_{z3}^* & h_{2z3} & z_{2z3} & w_{z3}^* w_{z3}^* & w_{z3}^* w_{z3}^* \frac{\lambda_5 + \lambda_6 - 4\lambda_7}{\sqrt{2}} \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} \\
    h_{2z3} & \lambda_5 + \lambda_6 - 2\lambda_7 & \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
    z_{2z3} & 2\lambda_7 & \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
    w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* \\
    w_{z3}^* & \frac{\lambda_5 + \lambda_6 - 4\lambda_7}{\sqrt{2}} & \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
\end{pmatrix},$$

$$\mathcal{G} = \begin{pmatrix}
    w_{z3}^* & h_{2z3} & z_{2z3} & w_{z3}^* w_{z3}^* & w_{z3}^* w_{z3}^* \frac{\lambda_5 + \lambda_6 - 4\lambda_7}{\sqrt{2}} \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} \\
    h_{2z3} & \lambda_5 + \lambda_6 - 2\lambda_7 & \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
    z_{2z3} & 2\lambda_7 & \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
    w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* & w_{z3}^* \\
    w_{z3}^* & \frac{\lambda_5 + \lambda_6 - 4\lambda_7}{\sqrt{2}} & \frac{\lambda_5 + \lambda_6 - 2\lambda_7}{\sqrt{2}} & \lambda_4 & -\lambda_4 & 0 \\
\end{pmatrix},$$

and

$$\mathcal{H} = \begin{pmatrix}
    3(\lambda_1 + \lambda_3) & 3(\lambda_1 + \lambda_3) & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 \\
    \lambda_1 + \lambda_3 & 3(\lambda_1 + \lambda_3) & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 \\
    \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 \\
    \lambda_1 - 2\lambda_2 - \lambda_3 & 3(\lambda_1 + \lambda_3) & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 \\
    \lambda_1 - 2\lambda_2 - \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 & \lambda_1 + \lambda_3 \\
\end{pmatrix}.$$
The eigenvalues of $E$ can be found to be $a_i^\pm (i = 1, \ldots, 6)$ which are listed in Eq. (37). Thus by obtaining the eigenvalues of $D$ and $E$ we get all the eighteen eigenvalues of $\mathcal{M}_{NC}^{(2)}$. Earlier we obtained the twelve eigenvalues of $\mathcal{M}_{NC}^{(1)}$. So we get all thirty eigenvalues of the $30 \times 30$ neutral channel S-matrix.

A.2 Charged Channels:

There will be $2 \cdot (3)^2 = 18$ charged two-particle states (CTPS) in the case of three Higgs doublets. That is why the charged channel S-matrix will be an $18 \times 18$ matrix. We write the basis of CTPS as,

$$\{w_1^+ h_2, w_1^+ h_3, w_1^+ z_2, w_1^+ z_3, w_2^+ h_1, w_2^+ z_1, w_3^+ h_1, w_3^+ z_1, w_1^+ z_2, w_2^+ h_2, w_2^+ h_3, w_2^+ z_2, w_3^+ h_2, w_3^+ h_3, w_3^+ z_2, w_3^+ z_3\}.$$

For reasons explained in the text before Eq. (52), this choice of basis will lead to a $(8\times8) \oplus (10\times10)$ block-diagonal S-matrix in the charged sector as follows:

$$\mathcal{M}_{CC} = \begin{pmatrix} \mathcal{J}_{8\times8} & 0_{8\times10} \\ 0_{10\times8} & \mathcal{K}_{10\times10} \end{pmatrix}.$$  (60)

Clearly if we can find the eigenvalues of the matrices $\mathcal{J}$ and $\mathcal{K}$ we get all the eigenvalues of $\mathcal{M}_{CC}$. The matrix $\mathcal{J}$ is given by,

$$\mathcal{J} = \begin{pmatrix} w_1^+ h_2 & w_1^+ h_3 & w_1^+ z_2 & w_1^+ z_3 & w_2^+ h_1 & w_2^+ h_3 & w_2^+ z_1 & w_2^+ z_3 \\ 2(\lambda_1 - \lambda_3) & \lambda_4 & 0 & 0 & 2\lambda_3 & 2i\lambda_2 & \lambda_4 & 0 \\ \lambda_4 & \lambda_5 & \lambda_4 & 0 & 0 & \frac{\lambda_6 + 2\lambda_7}{2} & -i(\lambda_6 - 2\lambda_7) & 0 \\ 0 & 0 & 2(\lambda_1 - \lambda_3) & \lambda_4 & -2i\lambda_2 & 2\lambda_3 & 0 & \frac{\lambda_4}{2} \\ \lambda_4 & \lambda_5 & 0 & \lambda_4 & 2(\lambda_1 - \lambda_3) & 0 & \lambda_4 & \frac{\lambda_4}{2} \\ 2\lambda_3 & 0 & 2i\lambda_2 & 0 & 2(\lambda_1 - \lambda_3) & 0 & \lambda_4 & 0 \\ -2i\lambda_2 & \lambda_4 & 0 & 0 & \frac{i(\lambda_6 - 2\lambda_7)}{2} & \lambda_4 & 0 & 0 \\ 0 & i(\lambda_6 - 2\lambda_7) & \frac{\lambda_6 + 2\lambda_7}{2} & 0 & 0 & \lambda_4 & 0 & \lambda_5 \\ \end{pmatrix}.$$

The eigenvalues of this matrix are $a_i^\pm (i = 1, 4)$ and $b_i$ ($i = 2, 4, 5, 6$) which are listed in Eq. (37). The matrix $\mathcal{K}$ can be written as,

$$\mathcal{K} = \begin{pmatrix} \mathcal{P}_{5\times5} & \mathcal{Q}_{5\times5} \\ \mathcal{Q}_{5\times5}^T & \mathcal{R}_{5\times5} \end{pmatrix},$$  (61)

where $\mathcal{P}$, $\mathcal{Q}$ and $\mathcal{R}$ are given by,

$$\mathcal{P} = \begin{pmatrix} w_1^+ h_1 & w_1^+ z_1 & w_2^+ h_2 & w_2^+ h_3 & w_2^+ z_2 \\ 2(\lambda_1 + \lambda_3) & 2\lambda_3 & 2i\lambda_2 & 0 & 2\lambda_3 \\ 0 & 2(\lambda_1 + \lambda_3) & 2i\lambda_2 & 0 & 2\lambda_3 \\ 2\lambda_3 & -2i\lambda_2 & 2(\lambda_1 + \lambda_3) & -\lambda_4 & 0 \\ 2i\lambda_2 & 0 & -\lambda_4 & \lambda_5 & 0 \\ \end{pmatrix},$$

$$\mathcal{Q} = \begin{pmatrix} w_1^+ h_1 & w_1^+ z_1 & w_2^+ h_2 & w_2^+ h_3 & w_2^+ z_2 \\ 0 & \lambda_4 & \frac{1}{2}(\lambda_6 + 2\lambda_7) & 0 & \frac{1}{2}(\lambda_6 - 2\lambda_7) \\ \lambda_4 & 0 & \frac{1}{2}(\lambda_6 - 2\lambda_7) & \lambda_4 & \frac{1}{2}(\lambda_6 + 2\lambda_7) \\ 0 & -\lambda_4 & \frac{1}{2}(\lambda_6 + 2\lambda_7) & 0 & \frac{1}{2}(\lambda_6 - 2\lambda_7) \\ \frac{1}{2}(\lambda_6 + 2\lambda_7) & \lambda_4 & 0 & \frac{1}{2}(\lambda_6 - 2\lambda_7) & 0 \\ -\lambda_4 & 0 & \frac{1}{2}(\lambda_6 - 2\lambda_7) & -\lambda_4 & \frac{1}{2}(\lambda_6 + 2\lambda_7) \\ \end{pmatrix}.$$
\[ Q^\dagger = \begin{pmatrix}
    w_{i3}^+ h_1 & w_{i3}^+ z_1 & w_{i3}^+ h_2 & w_{i3}^+ h_3 & w_{i3}^+ z_2 \\
    0 & \lambda_4 & 0 & 0 & -\lambda_4 \\
    \frac{1}{2}(\lambda_6 + 2\lambda_7) & 0 & \frac{1}{2}(\lambda_6 + 2\lambda_7) & 0 & \frac{1}{2}(\lambda_6 - 2\lambda_7) \\
    \frac{1}{2}(\lambda_6 - 2\lambda_7) & \lambda_4 & 0 & \frac{1}{2}(\lambda_6 - 2\lambda_7) & -\lambda_4 \\
\end{pmatrix}, \]

and,

\[ R = \begin{pmatrix}
    w_{i3}^+ z_3 & w_{i3}^+ h_2 & w_{i3}^+ h_3 & w_{i3}^+ z_2 & w_{i3}^+ z_3 \\
    \lambda_5 & 0 & 0 & \lambda_6 + 2\lambda_7 & 0 \\
    \frac{1}{2}(\lambda_6 - 2\lambda_7) & \lambda_5 & 0 & 0 & 0 \\
    0 & 0 & 0 & 2\lambda_8 & 0 \\
    \frac{1}{2}(\lambda_6 + 2\lambda_7) & 0 & 0 & 0 & 2\lambda_8 \\
\end{pmatrix}. \]

We find the eigenvalues of the matrix \( K \) to be \( a_i^\pm (i = 1, \ldots, 4) \), \( b_i (i = 2, 6) \) as listed in Eq. (37). Thus we get all the eigenvalues of the matrix \( \mathcal{M}_{CC} \).

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