

# Can one have significant deviations from leptonic $3 \times 3$ unitarity in the framework of type I seesaw mechanism?

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**Abstract** We address the question of deviations from  $3 \times 3$  unitarity of the leptonic mixing matrix showing that, in the framework of type I seesaw mechanism, one may have significant deviations from unitarity that can be detected at the next round of experiments while some of the heavy neutrino masses are sufficiently low to become within experimental reach. For that purpose we introduce a specially useful parametrisation that enables to control all deviations of unitarity through a single  $3 \times 3$  matrix, which we denote by  $X$  and which connects the mixing of the light and heavy neutrinos in the context of type I seesaw. We show that there is no need for the Yukawa couplings to be extremely suppressed. We present specific examples where deviations from  $3 \times 3$  unitarity are sufficiently small to conform to all the present stringent experimental bounds.

## 1 Introduction

The discovery of neutrino oscillations and at least two non-vanishing neutrino masses, provides clear evidence for Physics Beyond the Standard Model (SM). The simplest extension of the SM accommodating two non-vanishing neutrino masses involves the addition of at least two right-handed neutrinos. The most general gauge invariant Lagrangian includes a right-handed bare Majorana mass matrix  $M$ . As a result, the scale of  $M$  can be much larger than the electroweak scale, which leads to an elegant explanation for the smallness of neutrino masses, through the seesaw mechanism [1–5].

The seesaw mechanism necessarily implies violations from  $3 \times 3$  unitarity of the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) matrix, as well as Z-mediated lepton flavour violating couplings. The introduction of these heavy right-handed neutrinos can also have profound cosmological implications since they are a crucial component of the Leptogenesis mechanism to create the observed Baryon Asymmetry of the Universe (BAU) [6]. Leptogenesis is a very appealing scenario, for reviews see for example [7–13] but for heavy neutrinos with masses many orders of magnitude higher than the electroweak scale it is difficult or impossible to test it at low energies [14–16]. Furthermore, without a flavour model, CP violation at high energies, relevant for Leptogenesis, cannot be related to CP violation at low energies [17, 18]. This may be possible in the context of a flavour model, involving symmetries which allow to establish a connection between high and low energies [19–26].

At this stage, it should be emphasised that within the seesaw type I framework, the observed pattern of neutrino masses and mixing does not require that all the heavy neutrino masses be much larger than the electroweak scale. In this paper, we carefully examine the question of whether it is possible, within the seesaw type I mechanism, to have experimentally detectable violations of  $3 \times 3$  unitarity, taking into account the present experimental constraints. In particular, we address the following questions:

- (i) In the seesaw type I mechanism, is it possible to have significant deviations from  $3 \times 3$  unitarity of the leptonic mixing matrix? By significant, we mean deviations which are sufficiently small to conform to all present stringent experimental constraints on these deviations, but are sufficiently large to be detectable in the next round of experiments. These experimental constraints arise from bounds on rare processes.

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(ii) In the case the scenario described in (i) can indeed be realised within the framework of seesaw type I, what are the requirements on the pattern of heavy neutrino masses?

For definiteness, we will work in a framework where three right-handed neutrinos are added to the spectrum of the SM. Our analysis starts with the introduction of the unitary  $6 \times 6$  mixing matrix  $\mathcal{V}$ , characterising all the leptonic mixing. We write this  $6 \times 6$  mixing matrix in terms of four blocks of  $3 \times 3$  matrices. Using unitarity of  $\mathcal{V}$ , we show that the full matrix  $\mathcal{V}$  can be expressed in terms of only three blocks of  $3 \times 3$  matrices. Then we apply these results to the diagonalisation of the  $6 \times 6$  neutrino mass matrix, including both Dirac and Majorana mass terms. Through the use of a specially convenient exact parametrisation of the  $6 \times 6$  leptonic unitary mixing matrix, we evaluate deviations from  $3 \times 3$  unitarity and derive the maximum value of the lightest heavy neutrino mass which is required in order to generate significant deviations from unitarity in the framework of the seesaw type I mechanism.

The paper is organised as follows. In the next section, we review the seesaw mechanism, define our notation and introduce a specially convenient exact parametrisation of the  $6 \times 6$  leptonic mixing matrix  $\mathcal{V}$ . We evaluate the size of the deviations of  $3 \times 3$  unitarity in the present framework and derive a constraint on the magnitude of the mass of the heavy Majorana neutrinos, in order to have significant deviations of unitarity. Numerical examples are given in Sect. 3 and some of the derivations of our results are put in an Appendix. Finally we present our conclusions in the last section.

## 2 Deviations from unitarity in the leptonic sector

### 2.1 Type I seesaw mechanism

In the context of the Type I seesaw mechanism, with only three right-handed neutrinos added to the Lagrangian of the SM, the leptonic mass terms are given by:

$$\begin{aligned} \mathcal{L}_m &= -\left[ \bar{\nu}_L^0 m \nu_R^0 + \frac{1}{2} \nu_R^{0T} C M \nu_R^0 + \bar{l}_L^0 m_l l_R^0 \right] + h.c. \\ &= -\left[ \frac{1}{2} \bar{n}_L^T C \mathcal{M}^* n_L + \bar{l}_L^0 m_l l_R^0 \right] + h.c., \end{aligned} \tag{1}$$

There is no loss of generality in choosing a weak basis where  $m_l$  is already real and diagonal. The analysis that follows is performed in this basis. The neutrino mass matrix  $\mathcal{M}$  is a  $6 \times 6$  matrix and has the form:

$$\mathcal{M} = \begin{pmatrix} 0 & m \\ m^T & M \end{pmatrix}. \tag{2}$$

This matrix is diagonalised by the unitary transformation

$$\mathcal{V}^T \mathcal{M}^* \mathcal{V} = \mathcal{D} \quad \text{i.e.} \quad \mathcal{V}^\dagger \mathcal{M} = \mathcal{D} \mathcal{V}^T \tag{3}$$

where

$$\mathcal{D} = \begin{pmatrix} d & 0 \\ 0 & D \end{pmatrix} \tag{4}$$

with  $d = \text{diag.}(m_1, m_2, m_3)$  and  $D = \text{diag.}(M_1, M_2, M_3)$  denoting respectively, the light and the heavy Majorana neutrino masses. The unitary  $6 \times 6$  matrix  $\mathcal{V}$  is often denoted in the literature as:

$$\mathcal{V} = \begin{pmatrix} K & R \\ S & Z \end{pmatrix}, \tag{5}$$

where  $K, R, S$  and  $Z$  are  $3 \times 3$  matrices. For  $K$  and  $Z$  non singular, we may write

$$\mathcal{V} = \begin{pmatrix} K & 0 \\ 0 & Z \end{pmatrix} \begin{pmatrix} \mathbf{1} & Y \\ -X & \mathbf{1} \end{pmatrix}; \quad -X = Z^{-1}S; \quad Y = K^{-1}R \tag{6}$$

From the unitary relation  $\mathcal{V} \mathcal{V}^\dagger = \mathbf{1}_{(6 \times 6)}$ , we promptly conclude that

$$Y = X^\dagger. \tag{7}$$

The matrix  $\mathcal{V}$  can thus be written:

$$\mathcal{V} = \begin{pmatrix} K & K X^\dagger \\ -Z X & Z \end{pmatrix}. \tag{8}$$

We have thus made clear that the unitary  $6 \times 6$  matrix  $\mathcal{V}$  can be expressed in terms of three independent  $3 \times 3$  matrices. From the unitarity of  $\mathcal{V}$ , we obtain:

$$\begin{aligned} K (\mathbf{1} + X^\dagger X) K^\dagger &= \mathbf{1} \\ Z (\mathbf{1} + X X^\dagger) Z^\dagger &= \mathbf{1}, \end{aligned} \tag{9}$$

showing that the matrix  $X$  parametrizes the deviations from unitarity of the matrices  $K$  and  $Z$ . More explicitly:

$$\begin{aligned} K K^\dagger &= \mathbf{1} - K X^\dagger X K^\dagger \\ Z Z^\dagger &= \mathbf{1} - Z X X^\dagger Z^\dagger. \end{aligned} \tag{10}$$

From Eq. (3) we derive:

$$-X^\dagger Z^\dagger m^T = d K^T \tag{11}$$

$$K^\dagger m - X^\dagger Z^\dagger M = -d X^T Z^T \tag{12}$$

$$Z^\dagger m^T = D X^* K^T \tag{13}$$

$$X K^\dagger m + Z^\dagger M = D Z^T, \tag{14}$$

replacing  $Z^\dagger m^T$  from Eq. (13) into Eq. (11) we get

$$d = -X^T D X, \tag{15}$$

which implies that:

$$X = \pm i \sqrt{D^{-1}} O_c \sqrt{d}, \tag{16}$$

where  $O_c$  is a complex orthogonal matrix, i.e.,  $O_c^T O_c = \mathbb{1}$ , or explicitly:

$$|X_{ij}| = \left| (O_c)_{ij} \sqrt{\frac{m_j}{M_i}} \right|. \tag{17}$$

Note that Eq. (15) is equivalent to Eq. (2.30) derived in Ref. [17], which is an exact relation resulting from the existence of the zero  $3 \times 3$  block in the matrix  $\mathcal{M}$  of Eq. (2).

It should be stressed that the parametrisation of the  $6 \times 6$  unitary matrix  $\mathcal{V}$  given by Eq. (8) has the especial property of allowing to connect in a straightforward and simple way the masses of the light and the heavy neutrinos through an orthogonal complex matrix  $O_c$ , as can be seen from Eqs. (15) and (16). This is an important new result which plays a crucial rôle in our analysis.

Previously, in a variety of contexts, there have been various attempts at describing the possibility of having non-unitary lepton mixing [27,28]. The key point of our analysis is its generality. The parametrisation of Eq. (8) allows one to write the unitary  $6 \times 6$  mixing matrix  $\mathcal{V}$  in terms of two quasi-unitary matrices  $K$  and  $Z$  and a matrix  $X$  which controls the deviations from unitarity of both  $K$  and  $Z$ . This is explicitly shown in Eq. (10). The analysis we present here has the advantage of leading to a clearcut quantification of the phenomenological non-unitarity bounds in terms of the related  $6 \times 6$  lepton mixing matrix parameters. Another important point is the fact that, unlike in the case of Ref. [29], we do not assume conservation of lepton number. In the sequel, we shall also present a clear and straightforward relation between the non-unitary deviations and the scale of the neutrino Dirac mass matrix.

Since  $O_c$  is an orthogonal complex matrix, not all of its elements need to be small; furthermore, not all the  $M_i$  need to be much larger than the electroweak scale, in order for the seesaw mechanism to lead to naturally suppressed neutrino masses. These observations about the size of the elements of  $X$  are specially relevant in view of the fact that some of the important physical implications of the seesaw model depend crucially on  $X$ . In particular, the deviations from  $3 \times 3$  unitarity are controlled by  $X$ , as shown in Eq. (10).

Given the importance of the matrix  $X$ , one may ask whether it is possible to write the  $6 \times 6$  unitary matrix  $\mathcal{V}$  in terms of  $3 \times 3$  blocks, where only  $3 \times 3$  unitary matrices enter, together with the matrix  $X$ . In the Appendix, we show that this is indeed possible, and that the matrix  $\mathcal{V}$  can be written:

$$\begin{aligned} \mathcal{V} &= \begin{pmatrix} K & R \\ S & Z \end{pmatrix} \\ &= \begin{pmatrix} \Omega \left( \sqrt{\mathbb{1} + X^\dagger X} \right)^{-1} & \Omega \left( \sqrt{\mathbb{1} + X^\dagger X} \right)^{-1} X^\dagger \\ -\Sigma \left( \sqrt{\mathbb{1} + X X^\dagger} \right)^{-1} X & \Sigma \left( \sqrt{\mathbb{1} + X X^\dagger} \right)^{-1} \end{pmatrix}, \end{aligned} \tag{18}$$

where  $\Omega$  and  $\Sigma$  are  $3 \times 3$  unitary matrices given by:

$$\Omega = U_K U^\dagger \quad \Sigma = W_Z W^\dagger, \tag{19}$$

and  $U, W$  are the unitary matrices that diagonalise respectively  $X^\dagger X$  and  $X X^\dagger$ :

$$U^\dagger X^\dagger X U = d_X^2; \quad W^\dagger X X^\dagger W = d_X^2. \tag{20}$$

It is also shown in the Appendix, that  $U_K$  and  $W_Z$  defined by:

$$U_K \equiv K U \sqrt{(\mathbb{1} + d_X^2)} \quad W_Z \equiv Z W \sqrt{(\mathbb{1} + d_X^2)}, \tag{21}$$

are in fact unitary matrices.

As will be explained in the next section, this will allow us, in our analysis, to trade the matrix  $K$  by the combination  $U_K U^\dagger$  which we identify as the best fit for  $U_{PMNS}$  derived under the assumption of unitarity, multiplied by the remaining factor that parametrises the deviations from unitarity.

### 2.2 On the size of deviations from unitarity

In the framework of the type I seesaw, it is the block  $K$  of the matrix  $\mathcal{V}$  that takes the rôle played by  $U_{PMNS}$  matrix at low energies in models with only Dirac-type neutrino masses. Clearly, in this framework,  $K$  is no longer a unitary matrix. However, present neutrino experiments are putting stringent constraints on the deviations from unitarity. In our search for significant deviations from unitarity of  $K$ , we must make appropriate choices for the matrix  $X$  in order to comply with the experimental bounds, while at the same time obtain deviations that are sizeable enough to be detected experimentally in the near future. Our aim is to show how one can achieve this result with at least one of the heavy neutrinos with a mass at the TeV scale, without requiring unnaturally small Yukawa couplings and still have light neutrino masses not exceeding one eV.

Deviations from unitarity [30–35] of  $K$  have been parametrised as the product of an Hermitian matrix by a unitary matrix [34]:

$$K = (\mathbb{1} - \eta)V, \tag{22}$$

where  $\eta$  is an Hermitian matrix with small entries. In order to identify the different components of our matrix  $K$ , given

in Eq. (18), with the parametrisation of Eq. (22) we rewrite  $K$  as:

$$K = U_K U^\dagger \left( \sqrt{\mathbb{I} + X^\dagger X} \right)^{-1} = \left[ U_K U^\dagger \left( \sqrt{\mathbb{I} + X^\dagger X} \right)^{-1} U U_K^\dagger \right] U_K U^\dagger, \tag{23}$$

inside the square brackets we wrote the Hermitian matrix that we identify with  $(\mathbb{I} - \eta)$ , and which will parametrise the deviations from unitarity. The matrix  $V \equiv U_K U^\dagger$  is a unitarity matrix which is identified with  $U_{PMNS}$  obtained from the standard parametrisation [36] for a unitary matrix. One can also write:

$$\left[ U_K U^\dagger \left( \sqrt{\mathbb{I} + X^\dagger X} \right)^{-1} U U_K^\dagger \right] \equiv \left[ U_K \left( \sqrt{\mathbb{I} + d_X^2} \right)^{-1} U_K^\dagger \right], \tag{24}$$

where  $d_X^2$  is a  $3 \times 3$  diagonal matrix, introduced in Eq. (20). Identifying the second expression of Eq. (24) to  $(\mathbb{I} - \eta)$  we derive:

$$\eta = \mathbb{I} - U_K \left( \sqrt{\mathbb{I} + d_X^2} \right)^{-1} U_K^\dagger \approx \frac{1}{2} U_K d_X^2 U_K^\dagger, \tag{25}$$

for small  $d_X^2$ . The matrix  $U_{PMNS}$  is then fixed making use of the present best fit values obtained from a global analysis based on the assumption of unitarity. As pointed out in [34], from the phenomenological point of view it is very useful to parametrise  $K$  with the unitary matrix on the right, due to the fact that experimentally it is not possible to determine which physical light neutrino is produced, and therefore, one must sum over the neutrino indices. As a result, most observables depend on  $KK^\dagger$  which depends on the following combination:

$$\left( KK^\dagger \right)_{\alpha\beta} = \delta_{\alpha\beta} - 2\eta_{\alpha\beta} + \mathcal{O} \left( \eta_{\alpha\beta}^2 \right). \tag{26}$$

The standard parametrisation for  $U_{PMNS}$  is given by [36]:

$$U_{PMNS} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix} \cdot P, \tag{27}$$

with  $P$  given by

$$P = \text{diag} \left( 1, e^{i\alpha_{21}}, e^{i\alpha_{31}} \right) \tag{28}$$

where  $c_{ij} = \cos \theta_{ij}$ ,  $s_{ij} = \sin \theta_{ij}$  and  $\delta$  is a Dirac-type CP violating phase, while  $\alpha_{21}, \alpha_{31}$  denote Majorana phases. Neutrino oscillation experiments are not sensitive to these factorisable phases.

**Table 1** Neutrino oscillation parameter summary from [37]. For  $\Delta m_{31}^2$ ,  $\sin^2 \theta_{23}$ ,  $\sin^2 \theta_{13}$ , and  $\delta$  the upper (lower) row corresponds to normal (inverted) neutrino mass hierarchy. <sup>a</sup>There is a local minimum in the second octant, at  $\sin^2 \theta_{23} = 0.596$  with  $\Delta\chi^2 = 2.08$  with respect to the global minimum. <sup>b</sup>There is a local minimum in the first octant, at  $\sin^2 \theta_{23} = 0.426$  with  $\Delta\chi^2 = 1.68$  with respect to the global minimum for IO

Parameter	Best fit	1 $\sigma$ range
$\Delta m_{21}^2$ [ $10^{-5} eV^2$ ]	7.56	7.37–7.75
$ \Delta m_{31}^2 $ [ $10^{-3} eV^2$ ](NO)	2.55	2.41–2.59
$ \Delta m_{31}^2 $ [ $10^{-3} eV^2$ ](IO)	2.49	2.45–2.53
$\sin^2 \theta_{12}$	0.321	0.305–0.339
$\sin^2 \theta_{23}$ (NO)	0.430	0.412–0.450 <sup>a</sup>
$\sin^2 \theta_{23}$ (IO)	0.596	0.576–0.614 <sup>b</sup>
$\sin^2 \theta_{13}$ (NO)	0.02155	0.02080–0.02245
$\sin^2 \theta_{13}$ (IO)	0.02140	0.02055–0.02222
$\delta$ (NO)	1.40 $\pi$	1.20–1.71 $\pi$
$\delta$ (IO)	1.44 $\pi$	1.70–1.21 $\pi$

There are several groups performing global phenomenological fits on  $\theta_{12}, \theta_{23}, \theta_{13}$  and  $\delta$ , as well as on neutrino mass differences [37–39].

The specific bounds vary slightly from group to group. For definiteness we present in Table 1 the present bounds on neutrino masses and leptonic mixing from [37]. The quantities  $\Delta m_{ij}^2$  are defined by  $(m_i^2 - m_j^2)$ .

In Ref. [34] global constraints are derived on the matrix  $\eta$  through a fit of twenty eight observables including the  $W$  boson mass, the effective mixing weak angle  $\theta_W$ , several ratios of  $Z$  fermionic decays, the invisible width of the  $Z$ , several ratios of weak decays constraining EW universality, weak decays constraining CKM unitarity and some radiative lepton flavour violating (LFV) processes. The final result is translated into:

$$|2\eta_{\alpha\beta}| \leq \begin{pmatrix} 2.5 \times 10^{-3} & 2.4 \times 10^{-5} & 2.7 \times 10^{-3} \\ 2.4 \times 10^{-5} & 4.0 \times 10^{-4} & 1.2 \times 10^{-3} \\ 2.7 \times 10^{-3} & 1.2 \times 10^{-3} & 5.6 \times 10^{-3} \end{pmatrix}. \tag{29}$$

Ref. [34] also compares these bounds with those of previous studies [33,40], pointing out that in general there is good agreement. Variations in the scale of the masses of the heavy neutrinos lead to small effects and therefore, do not significantly change our analysis. In view of the smallness of the entries of this matrix one can infer from Eq. (26) that the deviations from unitarity of the matrix  $K$  are very much constrained.

### 2.3 The elements of the neutrino Dirac mass matrix $m$ and deviations from unitarity

In this subsection, we show that there is a correlation among:

- The size of deviations from unitarity of the  $3 \times 3$  leptonic mixing matrix.
- The mass of the lightest heavy neutrino.

From Eq. (13) we get

$$m = K X^\dagger D Z^{*-1}, \tag{30}$$

the experimental fact that  $K$  is almost unitary implies that  $Z$  is also almost unitary. Therefore the Dirac mass matrix  $m$  is of the same order as  $X$  times  $D$ . Notice that the scale of  $D$  may be of the order of the top quark mass, so that indeed the Yukawa couplings need not be extremely small.

The elements of the neutrino Dirac mass matrix  $m$  are connected to the deviations from unitarity of the  $3 \times 3$  leptonic mixing matrix. From Eq. (30) together with Eqs. (21), (23) and (24), we obtain:

$$m = U_K \left( \sqrt{\mathbf{1} + d_X^2} \right)^{-1} d_X W^\dagger D W^* \left( \sqrt{\mathbf{1} + d_X^2} \right) W_Z^T, \tag{31}$$

where we have used  $d_X = W^\dagger X U$  from Eq. (20). Thus, we find

$$\begin{aligned} Tr [mm^\dagger] &= Tr \left[ \left( \sqrt{\mathbf{1} + d_X^2} \right)^{-1} d_X W^\dagger D W^* \right. \\ &\quad \left. \times \left( \mathbf{1} + d_X^2 \right) W^T D W d_X \left( \sqrt{\mathbf{1} + d_X^2} \right)^{-1} \right] \end{aligned} \tag{32}$$

As previously emphasised, deviations from  $3 \times 3$  unitarity in  $U_{PMNS}$  are controlled by the matrix  $X$ , as it is clear from Eq. (10). For  $X = 0$ , there are no deviations from unitarity. Small deviations from unitarity correspond to  $d_X$  small and, in that case, one has to a very good approximation,

$$Tr [mm^\dagger] = Tr [d_X W^\dagger D^2 W d_X], \tag{33}$$

which can be written as:

$$\begin{aligned} Tr [mm^\dagger] &= d_{X_1}^2 \left( M_1^2 |W_{11}|^2 + M_2^2 |W_{21}|^2 + M_3^2 |W_{31}|^2 \right) \\ &\quad + d_{X_2}^2 \left( M_1^2 |W_{12}|^2 + M_2^2 |W_{22}|^2 + M_3^2 |W_{32}|^2 \right) \\ &\quad + d_{X_3}^2 \left( M_1^2 |W_{13}|^2 + M_2^2 |W_{23}|^2 + M_3^2 |W_{33}|^2 \right). \end{aligned} \tag{34}$$

It can be shown that, using the properties of orthogonal complex matrices, only one of the  $d_{X_i}$ , which we take for definiteness as  $d_{X_3}$ , can have a significant value (e.g.  $d_{X_3} \approx 10^{-2}$ ), while the other two are negligible. In fact from the eigenvalue equation of  $X$  we find:

$$\begin{aligned} d_{X_1}^2 d_{X_2}^2 d_{X_3}^2 &= \frac{m_1 m_2 m_3}{M_1 M_2 M_3} \\ \frac{d_{X_1}^2 d_{X_2}^2 + d_{X_1}^2 d_{X_3}^2 + d_{X_2}^2 d_{X_3}^2}{d_{X_1}^2 + d_{X_2}^2 + d_{X_3}^2} &\lesssim O\left(\frac{m_3}{M_1}\right) \end{aligned} \tag{35}$$

choosing  $d_{X_3}^2$  large enough to be experimentally relevant forces the other two eigenvalues to be extremely small.

Thus, we find in good approximation

$$Tr [mm^\dagger] = d_{X_3}^2 \left( M_1^2 |W_{13}|^2 + M_2^2 |W_{23}|^2 + M_3^2 |W_{33}|^2 \right) \tag{36}$$

or using the unitarity of  $W$

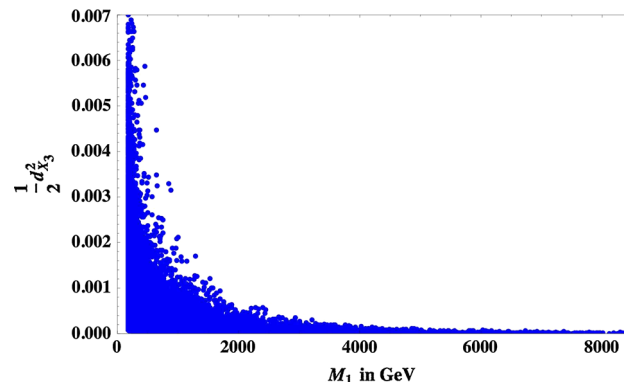
$$\begin{aligned} Tr [mm^\dagger] &= d_{X_3}^2 M_1^2 \left( 1 + \left( \frac{M_2^2}{M_1^2} - 1 \right) |W_{23}|^2 \right. \\ &\quad \left. + \left( \frac{M_3^2}{M_1^2} - 1 \right) |W_{33}|^2 \right) \end{aligned} \tag{37}$$

which, with the choice  $M_3 \geq M_2 \geq M_1$ , leads to

$$d_{X_3}^2 M_1^2 \leq Tr [mm^\dagger] = \sum_{i,j} |m_{ij}|^2 \tag{38}$$

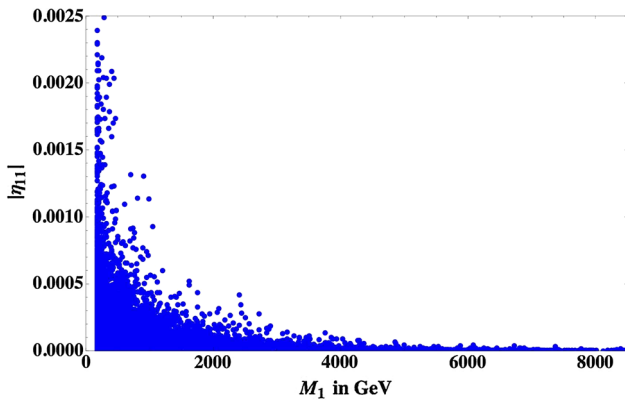
From Eq. (38), it is clear that for significant values of  $d_{X_3}$ ,  $M_1$  cannot be too large in order to avoid a too large value of  $Tr [mm^\dagger]$ , which in turn would imply that at least one of the  $|m_{ij}|^2$  is too large. This can be seen in both Fig. 1 and Fig. 3 where we plot  $\frac{1}{2}d_{X_3}^2$  versus  $M_1$ . Significant values of  $d_{X_3}^2$  can only be obtained for  $M_1 \leq 1 - 2$  TeV.

In all our plots, we require  $Tr [mm^\dagger] \leq m_t^2$ . We consider the case of normal ordering and vary over the values of light neutrinos masses  $m_i$ , up to  $m_3 = 0.5$  eV. Concerning the heavy Majorana masses  $M_i$ , we allow  $M_3$  to reach values of the order of  $10^4 m_t$  and allow for all possible forms of  $O_c$ . In Figs. 1, 2 we impose the condition that  $|\eta_{12}| \leq 10^{-4}$ , while in Figs. 3, 4, we chose  $|\eta_{12}| \leq 2 \times 10^{-5}$ .

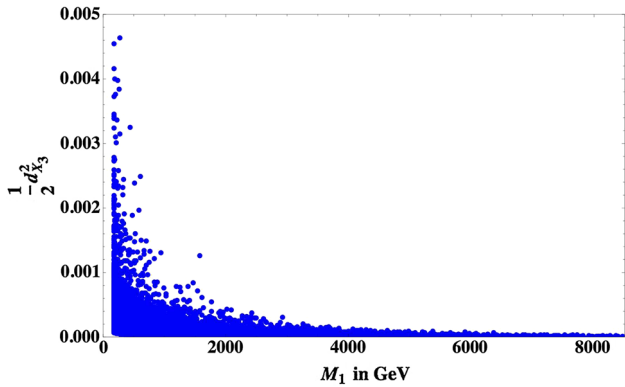


**Fig. 1** Maximum deviations from unitarity as a function of  $M_1$ , generated under the condition that  $Tr(mm^\dagger) \leq m_t^2$  and  $|\eta_{12}| \leq 10^{-4}$

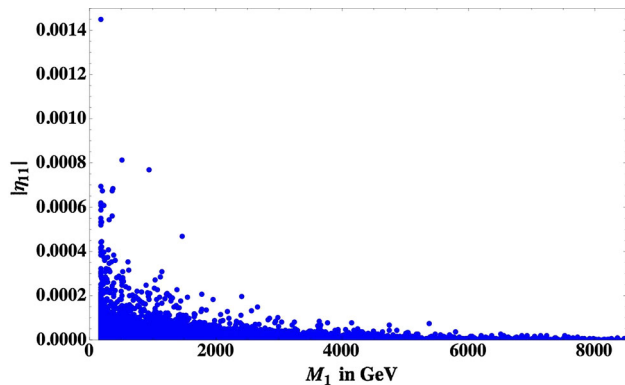




**Fig. 2**  $|\eta_{11}|$  deviations from unitarity as a function of  $M_1$ , generated under the condition that  $\text{Tr}(mm^\dagger) \leq m_\tau^2$  and  $|\eta_{12}| \leq 10^{-4}$



**Fig. 3** Maximum deviations from unitarity as a function of  $M_1$ , generated under the condition that  $\text{Tr}(mm^\dagger) \leq m_\tau^2$  and  $|\eta_{12}| \leq 2 \times 10^{-5}$



**Fig. 4**  $|\eta_{11}|$  deviations from unitarity as a function of  $M_1$ , generated under the condition that  $\text{Tr}(mm^\dagger) \leq m_\tau^2$  and  $|\eta_{12}| \leq 2 \times 10^{-5}$

In Figs. 2, 4, we also plot the  $|\eta_{11}|$  deviations from unitarity.

### 3 Numerical examples

In this section, we present some illustrative results of our numerical analysis showing that it is possible to obtain the

observed pattern of neutrino masses and mixing without requiring that all masses of the heavy Majorana neutrinos,  $M_i$ , be much larger than the electroweak scale. We have realistic examples even when all the three heavy neutrinos have masses below 2 TeV. One might expect that lowering the scale of the heavy neutrino masses would result in the need for extremely small Yukawa couplings for the Dirac mass terms, thus defeating the rationale for the seesaw mechanism. However, this is not the case and, to illustrate, we include for each example the corresponding moduli of the entries of the neutrino Dirac mass matrices  $m$  and the trace of the product  $mm^\dagger$ .

Our strategy is to fix the matrix  $X$  by choosing the matrices  $d, O_c$  and  $D$ , with  $d$  and  $D$  denoting the masses of the physical neutrinos. This immediately determines  $d_X^2, U$  and  $W$  and the deviations from unitarity of  $K$  and  $Z$ . Next we chose  $U_K$  in such a way that the block  $K$  falls within the experimental limits. The form of  $Z$  still depends on  $W_Z$  which can still be freely chosen. Since we have no experimental evidence constraining this block of  $\mathcal{V}$  we choose, for simplicity,  $W_Z$  equal to the identity, in some cases involving permutations, as explained in what follows.

In Table 2, we include examples with normal ordering of light neutrino masses, for a particular fixed value of these three masses, common to all examples. We consider three different hierarchies for the heavy Majorana neutrino masses  $M_i$ . For each choice of heavy neutrino mass hierarchy we give two examples, where we vary the matrix  $O_c$ . The other set of free parameters in our analysis are the Majorana-type phases entering in the choice of matrix  $\Omega$ .

In the first four examples given in Table 2 the orthogonal complex matrix is of the form:

$$O_c = \begin{pmatrix} 0 & \sqrt{x^2+1} & i x \\ 0 & i x & -\sqrt{x^2+1} \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \cos \tau & 0 & \sin \tau \\ 0 & 1 & 0 \\ -\sin \tau & 0 & \cos \tau \end{pmatrix}, \tag{39}$$

While in the last two examples given in Table 2 the orthogonal complex matrix is of the form:

$$O_c = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \sqrt{x^2+1} & i x \\ 0 & i x & -\sqrt{x^2+1} \\ 1 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} \cos \tau & 0 & \sin \tau \\ 0 & 1 & 0 \\ -\sin \tau & 0 & \cos \tau \end{pmatrix} \tag{40}$$

with different choices of  $x$  and  $\tau$  for the different cases, respectively:

**Table 2** Examples of deviations from unitarity, for the case of NO, with light neutrino masses  $m_1 = 0.005050 eV$ ,  $m_2 = 0.01005 eV$ ,  $m_3 = 0.05075 eV$ . The deviations from unitarity are expressed by the Hermitian matrix  $\eta$ . We consider three different hierarchies for the heavy Majorana neutrino masses  $M_i$ . For each hierarchy we give two examples, where we vary the choice of the matrix  $X$ . The third column contains the Dirac-type neutrino mass matrix, expressed in GeV units, and the fifth one contains the Majorana-type neutrino mass matrix, expressed in units of the top quark mass. The fourth column contains the trace of the product  $mm^\dagger$  in units of the squared top quark mass

Heavy neutrino masses	$ \eta $	$ m (GeV)$	$\text{tr}(mm^\dagger)(m_t^2)$	$ M (m_t)$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 9 m_t \end{pmatrix}$	$\begin{pmatrix} 1.12 \times 10^{-3} & . & . \\ . & 7.11 \times 10^{-8} & . \\ . & . & 1.65 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 24.6 & 6.88 \times 10^{-11} & 2.71 \times 10^{-5} \\ 0.196 & 3.43 \times 10^{-10} & 1.69 \times 10^{-4} \\ 29.9 & 3.03 \times 10^{-10} & 1.49 \times 10^{-4} \end{pmatrix}$	0.0497	$\begin{pmatrix} 9.99 \times 10^{-8} & 2.99 & 7.68 \times 10^{-6} \\ 2.99 & 1.99 \times 10^{-11} & 7.66 \times 10^{-6} \\ 7.68 \times 10^{-6} & 7.66 \times 10^{-6} & 8.99 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 9 m_t \end{pmatrix}$	$\begin{pmatrix} 5.43 \times 10^{-7} & . & . \\ . & 1.69 \times 10^{-4} & . \\ . & . & 1.86 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 0.542 & 1.21 \times 10^{-10} & 4.92 \times 10^{-5} \\ 9.57 & 3.69 \times 10^{-10} & 1.85 \times 10^{-4} \\ 31.78 & 3.41 \times 10^{-10} & 1.32 \times 10^{-4} \end{pmatrix}$	0.0366	$\begin{pmatrix} 1.00 \times 10^{-7} & 2.99 & 8.72 \times 10^{-6} \\ 2.99 & 2.40 \times 10^{-11} & 8.70 \times 10^{-6} \\ 8.72 \times 10^{-6} & 8.70 \times 10^{-6} & 8.99 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 100 m_t \end{pmatrix}$	$\begin{pmatrix} 1.12 \times 10^{-3} & . & . \\ . & 7.11 \times 10^{-8} & . \\ . & . & 1.65 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 24.6 & 6.88 \times 10^{-11} & 5.40 \times 10^{-5} \\ 0.196 & 3.43 \times 10^{-10} & 5.61 \times 10^{-4} \\ 29.9 & 3.03 \times 10^{-10} & 6.11 \times 10^{-4} \end{pmatrix}$	0.0497	$\begin{pmatrix} 1.00 \times 10^{-7} & 2.99 & 3.73 \times 10^{-5} \\ 2.99 & 1.99 \times 10^{-11} & 3.72 \times 10^{-5} \\ 3.73 \times 10^{-5} & 3.72 \times 10^{-5} & 99.9 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 100 m_t \end{pmatrix}$	$\begin{pmatrix} 5.43 \times 10^{-7} & . & . \\ . & 1.69 \times 10^{-4} & . \\ . & . & 1.86 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 0.542 & 1.21 \times 10^{-10} & 1.64 \times 10^{-4} \\ 9.57 & 3.69 \times 10^{-10} & 6.02 \times 10^{-4} \\ 31.8 & 3.41 \times 10^{-10} & 5.72 \times 10^{-4} \end{pmatrix}$	0.0366	$\begin{pmatrix} 1.00 \times 10^{-7} & 2.99 & 4.23 \times 10^{-5} \\ 2.99 & 2.40 \times 10^{-11} & 4.22 \times 10^{-5} \\ 4.23 \times 10^{-5} & 4.22 \times 10^{-5} & 99.9 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = 9 m_t \\ M_3 = (9 + 1 \times 10^{-7}) m_t \end{pmatrix}$	$\begin{pmatrix} 1.12 \times 10^{-3} & . & . \\ . & 7.11 \times 10^{-8} & . \\ . & . & 1.65 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 73.8 & 6.89 \times 10^{-11} & 2.73 \times 10^{-5} \\ 0.589 & 3.43 \times 10^{-10} & 9.70 \times 10^{-5} \\ 89.6 & 3.03 \times 10^{-10} & 1.33 \times 10^{-4} \end{pmatrix}$	0.447	$\begin{pmatrix} 1.00 \times 10^{-7} & 8.97 & 2.01 \times 10^{-5} \\ 8.97 & 1.85 \times 10^{-11} & 8.85 \times 10^{-6} \\ 2.01 \times 10^{-5} & 8.85 \times 10^{-6} & 2.99 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = 9 m_t \\ M_3 = (9 + 1 \times 10^{-7}) m_t \end{pmatrix}$	$\begin{pmatrix} 5.23 \times 10^{-7} & . & . \\ . & 1.62 \times 10^{-4} & . \\ . & . & 1.80 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 1.60 & 1.23 \times 10^{-10} & 2.85 \times 10^{-5} \\ 28.2 & 3.75 \times 10^{-10} & 1.02 \times 10^{-4} \\ 93.6 & 3.47 \times 10^{-10} & 1.29 \times 10^{-4} \end{pmatrix}$	0.317	$\begin{pmatrix} 1.00 \times 10^{-7} & 8.98 & 2.40 \times 10^{-5} \\ 8.98 & 2.49 \times 10^{-11} & 1.04 \times 10^{-5} \\ 2.40 \times 10^{-5} & 1.04 \times 10^{-5} & 2.99 \end{pmatrix}$

**Table 3** Examples of deviations from unitarity, for the case of IO, with light neutrino masses  $m_1 = 0.05064 eV$ ,  $m_2 = 0.05138 eV$ ,  $m_3 = 0.00864 eV$ . The deviations from unitarity are expressed by the Hermitian matrix  $\eta$ . We consider three different hierarchies for the heavy Majorana neutrino masses  $M_i$ . For each hierarchy we give two examples, where we vary the choice of the matrix  $X$ . The third column contains the Dirac-type neutrino mass matrix, expressed in GeV units, and the fifth one contains the Majorana-type neutrino mass matrix, expressed in units of the top quark mass. The fourth column contains the trace of the product  $mm^\dagger$  in units of the squared top quark mass

Heavy neutrino masses	$ \eta $	$ m (GeV)$	$\text{tr}(mm^\dagger)(m_t^2)$	$ M (m_t)$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 9 m_t \end{pmatrix}$	$\begin{pmatrix} 1.18 \times 10^{-3} & . & . \\ . & 8.50 \times 10^{-8} & . \\ . & . & 1.22 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 25.2 & 5.41 \times 10^{-10} & 1.67 \times 10^{-4} \\ 0.215 & 2.51 \times 10^{-10} & 1.59 \times 10^{-4} \\ 25.8 & 3.22 \times 10^{-10} & 1.64 \times 10^{-4} \end{pmatrix}$	0.0431	$\begin{pmatrix} 1.00 \times 10^{-7} & . & . \\ 2.99 & 5.01 \times 10^{-11} & . \\ 1.24 \times 10^{-7} & 1.23 \times 10^{-7} & 8.99 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 9 m_t \end{pmatrix}$	$\begin{pmatrix} 1.33 \times 10^{-7} & . & . \\ . & 2.16 \times 10^{-4} & . \\ . & . & 8.85 \times 10^{-4} \end{pmatrix}$	$\begin{pmatrix} 0.269 & 9.83 \times 10^{-10} & 1.63 \times 10^{-4} \\ 10.8 & 3.19 \times 10^{-10} & 1.17 \times 10^{-4} \\ 21.91 & 2.47 \times 10^{-10} & 9.96 \times 10^{-6} \end{pmatrix}$	0.0198	$\begin{pmatrix} 1.00 \times 10^{-7} & . & . \\ 2.99 & 4.04 \times 10^{-11} & . \\ 7.49 \times 10^{-7} & 7.48 \times 10^{-6} & 8.99 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 100 m_t \end{pmatrix}$	$\begin{pmatrix} 1.16 \times 10^{-3} & . & . \\ . & 8.43 \times 10^{-8} & . \\ . & . & 1.21 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 25.1 & 5.43 \times 10^{-10} & 5.56 \times 10^{-4} \\ 0.214 & 2.52 \times 10^{-10} & 5.31 \times 10^{-4} \\ 25.6 & 3.24 \times 10^{-10} & 5.47 \times 10^{-4} \end{pmatrix}$	0.0428	$\begin{pmatrix} 1.00 \times 10^{-7} & . & . \\ 2.99 & 5.05 \times 10^{-11} & . \\ 3.20 \times 10^{-7} & 3.19 \times 10^{-7} & 100 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = (3 + 1 \times 10^{-7}) m_t \\ M_3 = 100 m_t \end{pmatrix}$	$\begin{pmatrix} 1.33 \times 10^{-7} & . & . \\ . & 2.16 \times 10^{-4} & . \\ . & . & 8.85 \times 10^{-4} \end{pmatrix}$	$\begin{pmatrix} 0.269 & 9.83 \times 10^{-10} & 5.44 \times 10^{-4} \\ 10.8 & 3.19 \times 10^{-10} & 4.31 \times 10^{-4} \\ 21.9 & 2.47 \times 10^{-10} & 1.13 \times 10^{-4} \end{pmatrix}$	0.0198	$\begin{pmatrix} 1.00 \times 10^{-7} & . & . \\ 3.00 & 4.04 \times 10^{-11} & . \\ 3.63 \times 10^{-5} & 3.63 \times 10^{-5} & 99.9 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = 9 m_t \\ M_3 = (9 + 1 \times 10^{-7}) m_t \end{pmatrix}$	$\begin{pmatrix} 1.11 \times 10^{-3} & . & . \\ . & 8.05 \times 10^{-8} & . \\ . & . & 1.16 \times 10^{-3} \end{pmatrix}$	$\begin{pmatrix} 73.7 & 5.56 \times 10^{-10} & 9.63 \times 10^{-5} \\ 0.626 & 2.58 \times 10^{-10} & 9.20 \times 10^{-5} \\ 75.2 & 3.31 \times 10^{-10} & 9.48 \times 10^{-5} \end{pmatrix}$	0.367	$\begin{pmatrix} 1.00 \times 10^{-7} & . & . \\ 8.98 & 5.29 \times 10^{-11} & . \\ 1.68 \times 10^{-7} & 6.42 \times 10^{-8} & 2.99 \end{pmatrix}$
$\begin{pmatrix} M_1 = 3 m_t \\ M_2 = 9 m_t \\ M_3 = (9 + 1 \times 10^{-7}) m_t \end{pmatrix}$	$\begin{pmatrix} 1.32 \times 10^{-7} & . & . \\ . & 2.15 \times 10^{-4} & . \\ . & . & 8.80 \times 10^{-4} \end{pmatrix}$	$\begin{pmatrix} 0.804 & 9.85 \times 10^{-10} & 9.54 \times 10^{-5} \\ 32.4 & 3.20 \times 10^{-10} & 1.27 \times 10^{-4} \\ 65.5 & 2.48 \times 10^{-10} & 1.25 \times 10^{-4} \end{pmatrix}$	0.177	$\begin{pmatrix} 1.00 \times 10^{-7} & . & . \\ 8.99 & 4.06 \times 10^{-11} & . \\ 2.43 \times 10^{-5} & 2.08 \times 10^{-5} & 2.99 \end{pmatrix}$



$$\begin{aligned}
 x &= 2.40 \times 10^5 & \tau &= \frac{\pi}{2.9} \\
 x &= 2.12 \times 10^5 & \tau &= \frac{\pi}{2.8} \\
 x &= 2.40 \times 10^5 & \tau &= \frac{\pi}{2.9} \\
 x &= 2.12 \times 10^5 & \tau &= \frac{\pi}{2.8} \\
 x &= 4.16 \times 10^5 & \tau &= \frac{\pi}{2.9} \\
 x &= 3.60 \times 10^5 & \tau &= \frac{\pi}{2.8}
 \end{aligned}
 \tag{41}$$

The modulus of  $m$  is obtained from Eq. (30) and requires a choice for the  $W_Z$  matrix. This choice has implications for the entries of the blocks  $S$  and  $Z$  of the matrix  $\mathcal{V}$ . Since, at the moment, there are no direct experimental constraints on these entries, providing guidance for this choice, we made the simplest one, for both orderings, by fixing  $W_Z$  to be equal to the identity, in the first four examples. In the last two examples,

it was used  $W_Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ , such that the Majorana-type mass matrix,  $M$ , would be of the same form as the ones from the previous examples. With different choices of  $W_Z$  we could in principle homogenise the orders of magnitude of the entries of  $m$  so that all of the Yukawa couplings would be of the same order of magnitude or close.

In Table 3 we include examples with inverted ordering of light neutrino masses, for a particular fixed value of these three masses, common to all examples. We consider the same three different hierarchies for the heavy Majorana neutrino masses  $M_i$ , as in the cases of Table 2. For each choice of heavy neutrino mass hierarchy we give two examples, where we vary the matrix  $O_c$ . In the second and fourth examples of Table 3,  $O_c$  is of the form given by Eq. (39). In the sixth example of Table 3,  $O_c$  is of the form given by Eq. (40). In the first and third examples  $O_c$  is of the form:

$$O_c = \begin{pmatrix} \sqrt{x^2+1} & 0 & i x \\ i x & 0 & -\sqrt{x^2+1} \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \cos \tau & \sin \tau & 0 \\ -\sin \tau & \cos \tau & 0 \\ 0 & 0 & 1 \end{pmatrix},
 \tag{42}$$

While in the fifth example given in Table 3 the orthogonal complex matrix is of the form:

$$\begin{aligned}
 O_c &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{x^2+1} & 0 & i x \\ i x & 0 & -\sqrt{x^2+1} \\ 0 & 1 & 0 \end{pmatrix} \\
 &\times \begin{pmatrix} \cos \tau & \sin \tau & 0 \\ -\sin \tau & \cos \tau & 0 \\ 0 & 0 & 1 \end{pmatrix}
 \end{aligned}
 \tag{43}$$

The choices of  $x$  and  $\tau$  are respectively:

$$\begin{aligned}
 x &= 1.45 \times 10^5 & \tau &= \frac{\pi}{10} \\
 x &= 8.38 \times 10^4 & \tau &= \frac{\pi}{3.9} \\
 x &= 1.48 \times 10^5 & \tau &= \frac{\pi}{10} \\
 x &= 8.38 \times 10^4 & \tau &= \frac{\pi}{3.9} \\
 x &= 2.45 \times 10^5 & \tau &= \frac{\pi}{10} \\
 x &= 1.45 \times 10^5 & \tau &= \frac{\pi}{3.9}
 \end{aligned}
 \tag{44}$$

In all our examples the matrix  $X$  will have several entries of order at most  $10^{-2}$ .

### 4 Conclusions

We have studied the possibility of having significant deviations from  $3 \times 3$  unitarity of the leptonic mixing matrix in the framework of type-I seesaw mechanism. The analysis was done in the framework of an extension of the Standard Model where three right-handed neutrinos are added to the spectrum. We have shown that the  $6 \times 6$  unitary leptonic mixing matrix  $\mathcal{V}$  can be written in terms of two unitary  $3 \times 3$  matrices and a matrix denoted  $X$ , which controls the deviations from unitarity of the  $3 \times 3$  PMNS matrix. This parametrisation of the matrix  $\mathcal{V}$ , played a crucial role in showing that one may have significant deviations from  $3 \times 3$  unitarity while conforming to all present data on neutrino masses and mixing, as well as respecting all stringent bounds on deviations from  $3 \times 3$  unitarity of the PMNS matrix.

We have presented specific examples where the above deviations from unitarity are sufficiently large to have the potential for being observed at the next round of experiments. An important feature of our analysis is the fact that the mass of the lightest heavy sterile neutrino is, in principle, within experimental reach. This can be achieved without unnaturally small neutrino Yukawa couplings.

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**Appendix**

We can write the Hermitian matrices  $(\mathbb{I} + X^\dagger X)$  and  $(\mathbb{I} + X X^\dagger)$  as,

$$\mathbb{I} + X^\dagger X = U (\mathbb{I} + d_X^2) U^\dagger \tag{45}$$

$$\mathbb{I} + X X^\dagger = W (\mathbb{I} + d_X^2) W^\dagger,$$

where  $U$  and  $W$  are, by definition the unitary matrices which diagonalise the Hermitian matrices  $(\mathbb{I} + X^\dagger X)$  and  $(\mathbb{I} + X X^\dagger)$  respectively and  $d_X^2$  is a diagonal matrix. Inserting Eq. (45) into Eq. (9) we obtain:

$$\begin{aligned} K U (\mathbb{I} + d_X^2) U^\dagger K^\dagger &= K U \sqrt{(\mathbb{I} + d_X^2)} \cdot \sqrt{(\mathbb{I} + d_X^2)} U^\dagger K^\dagger = \mathbb{I} \\ Z W (\mathbb{I} + d_X^2) W^\dagger Z^\dagger &= Z W \sqrt{(\mathbb{I} + d_X^2)} \cdot \sqrt{(\mathbb{I} + d_X^2)} W^\dagger Z^\dagger = \mathbb{I} \end{aligned} \tag{46}$$

We therefore conclude that  $K U \sqrt{(\mathbb{I} + d_X^2)} = U_K$  and  $Z W \sqrt{(\mathbb{I} + d_X^2)} = W_Z$  are unitary matrices, and thus also that

$$\begin{aligned} K &= U_K \left( \sqrt{(\mathbb{I} + d_X^2)} \right)^{-1} U^\dagger \\ &= U_K U^\dagger \left( U \left( \sqrt{(\mathbb{I} + d_X^2)} \right)^{-1} U^\dagger \right) \\ Z &= W_Z \left( \sqrt{(\mathbb{I} + d_X^2)} \right)^{-1} W^\dagger \\ &= W_Z W^\dagger \left( W \left( \sqrt{(\mathbb{I} + d_X^2)} \right)^{-1} W^\dagger \right) \end{aligned} \tag{47}$$

or using the diagonalisation of the Hermitian matrices  $(\mathbb{I} + X^\dagger X)$  and  $(\mathbb{I} + X X^\dagger)$  in Eq.(45), we write this, as

$$\begin{aligned} K &= U_K \left( \sqrt{(\mathbb{I} + d_X^2)} \right)^{-1} U^\dagger = U_K U^\dagger \left( \sqrt{\mathbb{I} + X^\dagger X} \right)^{-1} \\ Z &= W_Z \left( \sqrt{(\mathbb{I} + d_X^2)} \right)^{-1} W^\dagger = W_Z W^\dagger \left( \sqrt{\mathbb{I} + X X^\dagger} \right)^{-1} \end{aligned} \tag{48}$$

which lead to Eq. (18).

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