Non-Unitarity of the lepton mixing matrix at the European spallation source

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If neutrinos get mass through the exchange of lepton mediators, as in seesaw schemes, the neutrino appearance probabilities in oscillation experiments are modified due to effective non-unitarity of the lepton mixing matrix. This also leads to new CP phases and an ambiguity in underpinning the “conventional” phase of the three-neutrino paradigm. We study the CP sensitivities of various setups based at the European spallation source neutrino super-beam (ESSnuSB) experiment in the presence of non-unitarity. We also examine its potential in constraining the associated new physics parameters.

I. INTRODUCTION

The discovery of neutrino oscillations [1, 2] has brought neutrinos to the center of particle physics. The current experimental data mainly converge into a consistent global picture in which the oscillation parameters are pretty well determined. However, three challenges still remain, namely, to determine the CP phase, the atmospheric octant and the ordering of the neutrino mass spectrum [3, 4]. These will be the target of a number of future experiments, such as DUNE [5]. A fourth item must be added to this list, namely probing the robustness of the interpretation, such as testing the unitarity of the lepton mixing matrix. This is crucial because it undermines the efforts of underpinning the CP phase $\delta_{\text{CP}}$ [6, 7].

This task is well justified also on theory grounds. Indeed, one of the most attractive ways to generate neutrino mass is through the mediation of heavy neutral leptons. While these emerge in many gauge extensions of the standard model, they can be postulated directly at the SU(3)$_c \otimes$ SU(2)$_L \otimes$ U(1)$_Y$ level, as the neutrino mass generation mediators.
This, in fact, provides the most general realization of the seesaw mechanism and many of its variants [8]. For generality here we focus exclusively on this case, namely, the standard $SU(3)_c \otimes SU(2)_L \otimes U(1)_Y$ seesaw mechanism. The resulting lepton mixing matrix is in general quite complex when compared with CKM mixing. First, lepton mixing contains extra phases that can not be eliminated by field redefinitions [8] and are therefore physical [9], crucially affecting lepton number violation processes. However, they do not affect conventional oscillations, so we will ignore them in what follows. On the other hand the lepton mixing matrix must in general take into account the admixture of the heavy lepton seesaw mediators with the light active neutrinos [10]. These are usually neglected, as the smallness of neutrino masses indicated by neutrino experiments suggests a very high seesaw scale.

Nonetheless, the seesaw mechanism can also be realized at low scales. The template for this is a scenario where two SM-singlet leptons are added sequentially, instead of just one. If lepton number symmetry is imposed, then all three active neutrinos are massless, as in the standard model. In contrast to the Standard Model, however, lepton flavor is violated, and similarly, leptonic CP symmetry. This shows that flavor and CP violation can exist in the leptonic weak interaction despite the masslessness of neutrinos, implying that such processes need not be suppressed by the small neutrino masses, and hence can be large [11–16].

Over such basic template one can build genuine “low-scale” realizations of the seesaw mechanism in which lepton number symmetry is restored at low, instead of high, values of the lepton number violation scale. The models are natural in t’Hooft sense, and lead to small, symmetry-protected neutrino masses. Such “low-scale” seesaw realizations include the inverse [17, 18] as well as the linear seesaw mechanisms [19–21]. In all of these we expect potentially sizeable unitarity violation in the leptonic weak interaction. This paper is dedicated to probing such effects at the European Spallation Source neutrino Super-Beam (ESSnuSB) experiment. Sensitivity studies to non-unitarity at other future long-baseline facilities can be found in Refs. [7, 22–24].

We briefly describe the theoretical framework for unitarity violation in the charged current (CC) leptonic weak interaction in Sec. II, and the matter three-neutrino oscillation probabilities with and without unitarity violation in Sect. III. Next, in Sec. IV, we describe the experimental setups of interest, and also present the details of the simulation we have performed. Our results are given in Sec. V and include our calculated ESSnuSB sensitivity to non-unitary (NU) neutrino mixing in Sec. VA, the CP violation discovery potential in the presence of unitarity violation is given in VB, and the CP reconstruction capabilities both for the standard phase as well as the seesaw phase of $\alpha_{21}$ in VC. Finally we briefly summarize in Sec. VI.
II. THEORETICAL FRAMEWORK

In the standard $3 \times 3$ oscillation picture, the neutrino mixing matrix is described symmetrically by a product of three mixing matrices

$$U = \omega_{23} \omega_{13} \omega_{12},$$

where each $\omega_{i,j}$ describes an effective $2 \times 2$ complex rotation, characterized by a mixing angle and its phase. This symmetrical form complements the original description [8] by specifying the most convenient factor ordering. In explicit form, the standard $3 \times 3$ leptonic mixing matrix is given by

$$U = \begin{pmatrix}
1 & 0 & 0 \\
0 & c_{23} & e^{-i\varphi_{23} s_{23}} \\
0 & -e^{i\varphi_{23} s_{23}} & c_{23}
\end{pmatrix}
\begin{pmatrix}
c_{13} & 0 & e^{-i\varphi_{13} s_{13}} \\
0 & 1 & 0 \\
-e^{i\varphi_{13} s_{13}} & 0 & c_{13}
\end{pmatrix}
\begin{pmatrix}
c_{12} & e^{-i\varphi_{12} s_{12}} \\
-c^{\ast}_{12} s_{12} & c_{12} & 0 \\
0 & 0 & 1
\end{pmatrix},$$

where $s_{ij} = \sin \theta_{ij}$, $c_{ij} = \cos \theta_{ij}$, and $\varphi_{ij}$ is the corresponding phase. One sees the appearance of two extra physical phases with no counterpart in the quark sector: the so-called Majorana phases [8]. Note that the above parameterization of the neutrino mixing matrix is equivalent to the oscillation-sensitive part of the PDG form [25] with $\varphi_{13} - \varphi_{12} - \varphi_{23} \equiv \delta_{CP}$ [26] so that when $\varphi_{12} = \varphi_{23} = 0$ one has $\varphi_{13} = \delta_{CP}$.

Apart from the presence of these new physical [9] phases, the leptonic CC interaction will in general also contain the mixing of neutral heavy leptons that mediate neutrino mass generation, as in the so-called type-I seesaw mechanism. These two facts make the mixing of massive neutrinos substantially richer in structure than that which describes the quark weak interactions [8]. As a result, in this general neutrino framework, $U_{n \times n}$ can be expressed as the product of the new physics (NP) piece, times the Standard Model (SM) piece

$$U_{n \times n} = U^{NP} U^{SM}. \quad (3)$$

Thinking in terms of the seesaw mechanism it is convenient to express the full $U$ matrix as four submatrices. Here we label them as in [27] ¹, i.e.

$$U_{n \times n} = \begin{pmatrix}
N & S \\
T & V
\end{pmatrix}. \quad (4)$$

Notice that we have a block, $N$, relating the light neutrino sector with the three active neutrino flavors. Here $V$ will be a $(n-3) \times (n-3)$ submatrix, while $S$ and $T$ will be, in general, rectangular matrices.

Clearly, in this general case, the full unitarity condition will take the form

$$NN^\dagger + SS^\dagger = I,$$
$$TT^\dagger + VV^\dagger = I. \quad (5)$$

¹ The form of the matrices $N, S, T$ and $V$ within the full seesaw expansion was given in Ref. [10]. They correspond, respectively, to $U_a, U_b, U_c$ and $U_d$ of Eqs. (2.8) and (3.5) of the above reference.
Therefore, the $3 \times 3$ matrix $N$ describing the mixing of light neutrinos will no longer be unitary. One can show [28] that in the most general case $N$ can be parametrized as

$$N = N^{NP} U^{3 \times 3} = \begin{pmatrix} \alpha_{11} & 0 & 0 \\ \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix} U^{3 \times 3},$$

(6)

where the diagonal $\alpha$’s are real and close to 1, while the off-diagonals are small but complex. Indeed, for any number of additional neutrino states, we will have for the diagonal entries of this matrix that

$$\alpha_{jj} = \prod_{i=4,n} \cos \theta_{ji},$$

(7)

with no sum over $j$. For small mixings, the non-diagonal entries are given as

$$\alpha_{ji} \simeq -\sum_{k=4,n} \theta_{jk} \theta_{ik} e^{-i(\varphi_{jk} - \varphi_{ik})}, \quad i < j.$$  

(8)

From this last expression, one can see that

$$|\alpha_{21}|^2 \leq \sum_{i=4}^{N} \left| \theta_{2i} \theta_{1i} e^{-i(\varphi_{2i} - \varphi_{1i})} \right|^2 = \sum_{i=4}^{N} \theta_{2i}^2 \theta_{1i}^2,$$

(9)

and similar equations for the other two non-diagonal terms. Using the triangle inequality, one can now derive the consistency relations

$$|\alpha_{ji}| \leq \sqrt{(1 - \alpha_{jj}^2)(1 - \alpha_{ii}^2)}.$$  

(10)

The muon neutrino appearance probability will be given as

$$P_{\mu e} = \alpha_{11}^2 |\alpha_{21}|^2 - 4 \sum_{j>i}^3 \mathrm{Re} \left[ N_{\mu j}^* N_{ej} N_{\mu i} N_{ei}^* \right] \sin^2 \left( \frac{\Delta m_{ji}^2 L}{4E} \right) + 2 \sum_{j>i}^3 \mathrm{Im} \left[ N_{\mu j}^* N_{ej} N_{\mu i} N_{ei}^* \right] \sin \left( \frac{\Delta m_{ji}^2 L}{2E} \right),$$

(11)

where $N$ is given in terms of the $\alpha$’s as in Eq. (6).

For the case of vacuum oscillations, the parameters characterizing unitarity violation in the $\mu$-$e$ sector are $\alpha_{11}$, $\alpha_{22}$, and $\alpha_{21}$. In the presence of matter effects, the appearance probability could also involve the third neutrino type, since the charged and neutral current potential will modify the effective form of the matrix $N$. The charged current potential for the non-unitary case will be given by

$$V_{CC}^{\alpha\beta} = \sqrt{2} G_F N_e \left( NN^\dagger \right)_{\alpha e} \left( NN^\dagger \right)_{e\beta},$$

(12)

For a general derivation of this expression without the assumption of small mixing angles see [29].
where $G_F$ is the Fermi constant and $N_e$ the number density of electrons in the medium. The matrix product will be written, in terms of the $\alpha$’s, as [7]:

$$ (NN^\dagger)_{\alpha\epsilon}(NN^\dagger)_{\epsilon\beta} = \alpha_{11}^2 \begin{pmatrix} \alpha_{11}^2 & \alpha_{11}\alpha_{21}^* \alpha_{11}\alpha_{31}^* \\ \alpha_{11}\alpha_{21} & |\alpha_{21}|^2 \alpha_{21}\alpha_{31}^* \\ \alpha_{11}\alpha_{31} & \alpha_{21}\alpha_{31}^* |\alpha_{31}|^2 \end{pmatrix}. $$

(13)

The corresponding potential for neutral currents will be

$$ V_{NC}^{\alpha\beta} = -\sqrt{2} G_F \frac{N_e}{2} \sum_\rho (NN^\dagger)_{\alpha\rho}(NN^\dagger)_{\rho\beta} = -\sqrt{2} G_F \frac{N_e}{2} \left[(NN^\dagger)^2\right]_{\alpha\beta}, $$

(14)

which, at leading order, takes the form [7]

$$ 
= \begin{pmatrix} \alpha_{11}^4 & \alpha_{11}\alpha_{21} (\alpha_{11}\alpha_{21} + \alpha_{22}) & \alpha_{11}\alpha_{31} (\alpha_{11}\alpha_{21} + \alpha_{33}) \\ \alpha_{11}\alpha_{21} (\alpha_{11}\alpha_{21} + \alpha_{22}) & \alpha_{22}^4 & \alpha_{22}\alpha_{32} (\alpha_{22}\alpha_{32} + \alpha_{33}) \\ \alpha_{11}\alpha_{31} (\alpha_{11}\alpha_{21} + \alpha_{33}) & \alpha_{22}\alpha_{32} (\alpha_{22}\alpha_{32} + \alpha_{33}) & \alpha_{33}^4 \end{pmatrix}. $$

Neglecting cubic terms in $\alpha_{21}$, $\sin \theta_{13}$, and $\Delta m_{21}^2$, one finds that, in the vacuum case limit, the main contribution to the conversion probability will be given by

$$ P_{\mu e} = (\alpha_{11}\alpha_{22})^2 P_{\mu e}^{3x3} + \alpha_{11}^2 \alpha_{22} |\alpha_{21}| P_{\mu e}^{I} + \alpha_{11}^2 |\alpha_{21}|^2, $$

(16)

where $P_{\mu e}^{3x3}$ denotes the usual three-neutrino conversion probability,

$$ P_{\mu e}^{3x3} = 4 \left[ \cos^2 \theta_{12} \cos^2 \theta_{23} \sin^2 \theta_{12} \sin^2 \left( \frac{\Delta m_{21}^2 L}{E_{\nu}} \right) \right] + \cos \theta_{12} \sin \theta_{13} \sin \frac{\Delta m_{21}^2 L}{2E_{\nu}} \sin \left( \frac{\Delta m_{31}^2 L}{4E_{\nu}} \right) \cos \left( \frac{\Delta m_{31}^2 L}{4E_{\nu}} + \delta_{CP} \right), $$

(17)

where $P_{\mu e}^{I}$ is the interference term

$$ P_{\mu e}^{I} = -2 \left[ \sin(2\theta_{13}) \sin \theta_{23} \sin \left( \frac{\Delta m_{31}^2 L}{4E_{\nu}} \right) \sin \left( \frac{\Delta m_{31}^2 L}{4E_{\nu}} + \delta_{CP} - \phi_{21} \right) \right] + \cos \theta_{13} \cos \theta_{23} \sin \frac{\Delta m_{21}^2 L}{2E_{\nu}} \phi_{21}, $$

(18)

with $\phi_{21} = \arg(\alpha_{21})$.

### III. THREE NEUTRINO OSCILLATION PROBABILITIES

Before coming to our numerical results, in this section we discuss the behaviour of the appearance and disappearance neutrino probabilities. To this end, we show in the left (right) panel of Fig. 1 the $\nu_\mu \rightarrow \nu_e$ ($\bar{\nu}_\mu \rightarrow \bar{\nu}_e$) oscillation probabilities as a function of the neutrino energy. The upper, middle, and lower panels correspond to 540 km, 360 km, and 200 km baselines, respectively. We show the conversion probability in the standard unitary framework as a solid line, while the
FIG. 1. The left panels represent the neutrino appearance probabilities for the unitary and non-unitary oscillation case, for three different baselines, as indicated. The right panels show the corresponding antineutrino probabilities. The neutrino and antineutrino $\nu_\mu$ fluxes divided by the squared of the baseline, and $\nu_e$-nucleus cross sections divided by the energy are also shown (in arbitrary units) as shaded regions.
\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
3\nu parameters & \text{sin}^2 \theta_{12} & \text{sin}^2 \theta_{13} & \text{sin}^2 \theta_{23} & \delta_{\text{CP}} & \Delta m_{12}^2 \text{eV}^2 & \Delta m_{23}^2 \text{eV}^2 \\
\hline
Benchmark values & 0.318 & 0.022 & 0.57 & [-180, 180] & 7.5 & 2.55 \\
Status & fixed & marginalized & marginalized & marginalized & fixed & marginalized \\
\hline
\end{tabular}
\caption{Benchmark values for the standard three-neutrino oscillation parameters taken from the current global fit analysis [3], along with their assumed marginalization status within our analyses, except $\delta_{\text{CP}}$. For simplicity, normal mass ordering (NO) has been assumed.}
\end{table}

dashed one represents the non unitary case. For the unitary case, we consider the values of the neutrino oscillation parameters given in Table I with $\delta_{\text{CP}} = -90^\circ$. For the non-unitary case, besides these values, we fix the non-unitary $\alpha$-parameters to be $\alpha_{11} = 0.97$, $\alpha_{22} = 0.99$, $\alpha_{33} = 1$, $|\alpha_{21}| = 0.02$, $\phi_{21} = 90^\circ$, $|\alpha_{31}| = 0$, and $|\alpha_{32}| = 0$. The expected resulting (anti)neutrino $\nu_\mu$ flux at the ESSnuSB, presented in the figures in arbitrary units, extend from 0.1 GeV to 1.0 GeV with a peak around 0.25 GeV. This peak lies close to the second oscillation maximum for baselines of 540 km and 360 km while, for the 200 km case, it lies in between the first and second oscillation maxima, see Table II. Notice that the total neutrino flux at the detector will decrease inversely proportional to the squared of the baseline distance. For completeness, we also show in Fig. 1 the energy dependence of the $\nu_e$-nucleus cross section [30, 31], $\sigma(E)$, divided by the energy.

The expected event number for the appearance signal will be given by the convolution of the cross section, the appearance probability and the neutrino energy spectrum at the detector, which depends on its distance to the source. For example, for a 200 km baseline, one can see from Fig. 1 that there is a minimum in the probability that almost coincides with the peak of the $\nu_\mu$ flux, thereby suppressing the neutrino signal. However, due to the different baselines, the total neutrino flux for the 200 km case will be approximately twice than for a 360 km baseline, and seven times the flux of the 540 km case. As a result, even at the probability minimum at 200 km as mentioned above, we expect more events than for the other two baselines. We will illustrate this point in more detail in the following sections.

\begin{table}
\centering
\begin{tabular}{|c|c|c|}
\hline
baseline (km) & 1st osc. max. (GeV) & 2nd osc. max. (GeV) \\
\hline
540 & 1.05 & 0.35 \\
360 & 0.70 & 0.23 \\
200 & 0.39 & 0.13 \\
\hline
\end{tabular}
\caption{Possible baselines of the ESSnuSB project [32–35], along with the corresponding values of the neutrino energy for the first and second oscillation maxima.}
\end{table}
IV. EXPERIMENTAL SETUP AND SIMULATION

In this section, we briefly discuss the experimental specifications of the ESSnuSB and DUNE setups used in this work, followed by a description of our simulation procedure.

A. Experimental setup options

The ESSnuSB project is a proposed accelerator neutrino experiment sourced at Lund (Sweden), where the ESS linac facility is currently under construction. The original ESSnuSB proposal was to use of a very intense proton beam of 2 GeV energy and an average beam power of 5 MW, resulting in $2.7 \times 10^{23}$ protons on target (POT) per year (208 effective days) [32–35]. Here we will adopt this configuration. It is expected that the future linac upgrade can increase the proton energy up to 3.6 GeV. The neutrino and antineutrino fluxes arising from the 2 GeV proton beam peak around 0.25 GeV [36]. These (anti)neutrinos will be detected by a 500 kton fiducial mass Water Cherenkov detector similar to the MEMPHYS project [37, 38]. Since the baseline of the far detector has not been finalized yet, we have considered in this work three possible baselines [32], which are 200 km, 360 km, and 540 km respectively. It has been shown in [32] that if the detector is placed in any of the existing mines in between 200 km to 600 km from the ESSnuSB site Lund, a $3\sigma$ evidence of CP violation could be achieved for 60% coverage of the full $\delta_{CP}$ range. Our simulation matches the event numbers of Table 3 and all other results given in [32]. In all the numerical results presented here, we have assumed 2 years of neutrino and 8 years of antineutrino running with an optimistic assumption of uncorrelated 5% signal normalization and 10% background normalization error for both neutrino and antineutrino appearance and disappearance channels, respectively. For more details about the accelerator facility, beamline design, detector and baseline positions of this setup, see [32]. Note that, while working on this paper, an updated analysis from the collaboration has come out [39]. Enhanced sensitivities to unitarity violation might be expected for the updated setup of the proposal. This highly potential and ambitious facility is expected to start taking data around the year 2030.

DUNE is a future long-baseline accelerator-based neutrino experiment with a baseline of 1300 km from the source at Fermilab to the far detector placed deep underground at the Sanford Laboratory site in South Dakota. DUNE will use a 40 kton LArTPC detector and a 120 GeV proton beam with 1.2 MW beam power resulting in $1.1 \times 10^{21}$ POT/year. For the numerical simulations, we have followed the experimental configurations provided by the collaboration in the Technical Design Report (TDR) [40, 41], assuming equal runtime of 3.5 years in neutrino and antineutrino mode, which results in 336 kton-MW-year exposure for the TDR setup. More details on the systematic errors, efficiencies and energy resolutions can be found in Refs. [41, 42].
B. Simulation procedure

In order to assess the statistical sensitivity of the ESSnuSB facility to neutrino oscillations, we have made use of the built-in $\chi^2$ function of the GLoBES package [43, 44], which incorporates the systematic errors through the pull terms [45]. To perform the non-unitarity analysis we have used the modified version of [46]. The total $\chi^2$ is a sum of all the contributions coming from different channels,

$$
\chi^2_{total} = \chi^2_{\nu_\mu \rightarrow \nu_e} + \chi^2_{\bar{\nu}_\mu \rightarrow \bar{\nu}_e} + \chi^2_{\nu_\mu \rightarrow \nu_\mu} + \chi^2_{\bar{\nu}_\mu \rightarrow \bar{\nu}_\mu}. 
$$

(19)

Unless stated otherwise, the benchmark choices of the standard three-neutrino unitary oscillation parameters and their marginalization status in our analysis are given in Table I. Our benchmark choices closely follow the current global fit analysis [3]. Following the same analysis, we have adopted a 1% uncertainty on the atmospheric mass-squared splitting $\Delta m_{31}^2$ and a 3.2% uncertainty on the reactor mixing angle $\sin^2 \theta_{13}$. We have freely marginalized over the atmospheric parameter $\sin^2 \theta_{23}$ from 0.35 to 0.65.

For the case of ESSnuSB, we have considered a line-averaged constant matter density $\rho = 2.8 \text{ g/cm}^3$ following the PREM profile [47, 48]. For DUNE, we have also assumed the same matter density but with a 5% uncertainty due to the longer baseline. For definiteness, we have assumed the currently preferred case of normal neutrino mass ordering (NO) throughout all of our analyses. Whenever appropriate, we have also marginalized over the NU parameters, along with their associated CP phases, implementing the current 3σ bounds shown in Table III. These come essentially from short-baseline oscillation searches such as from NOMAD [49, 50] and CHORUS [51, 52] and the long-baseline experiments T2K [53], NOvA [54] and, most importantly, MINOS/MINOS+ [55].

| NU parameters | $|\alpha_{21}|$ | $|\alpha_{31}|$ | $\alpha_{11}$ | $\alpha_{22}$ | $\alpha_{33}$ |
|---------------|----------------|----------------|-------------|-------------|-------------|
| 3σ bounds from Ref. [7] | $< 0.026$ | $< 0.13$ | $> 0.93$ | $> 0.95$ | $> 0.60$ |
| 3σ bounds from Ref. [29] | $< 0.025$ | $< 0.075$ | $> 0.93$ | $> 0.98$ | $> 0.72$ |

TABLE III. Current neutrino constraints on the non-unitary parameters from Refs. [7] and [29].

V. RESULTS

In this section we discuss in detail the numerical findings of our analyses, where we explore the sensitivity of the ESSnuSB facility to the non-unitary neutrino mixing, as well as the impact of non-unitarity on the measurement of the standard three-neutrino oscillation parameters, with emphasis on the CP-violating phase, $\delta_{CP}$. 
FIG. 2. ESSnuSB sensitivity to the non-unitarity scenario in the $(|\alpha_{21}|, \delta_{CP})$ plane. Left, middle, and right panels correspond to 540 km, 360 km, and 200 km baselines, respectively. Contours are shown at $1\sigma$, $2\sigma$, and $3\sigma$ C.L for 2 d.o.f. The red vertical lines indicate the current $3\sigma$ upper limit on $|\alpha_{21}|$ from neutrino data. We have assumed $\delta_{CP}(true) = -90^\circ$ and normal mass ordering. Note that the magenta star marked as benchmark in each panel has been used later to produce dashed spectra in the upper panel of Fig. 3.

A. Probing non-unitary neutrino mixing at ESSnuSB

We start our discussion from Fig. 2, where we show the ESSnuSB sensitivity to non-unitarity in the $(|\alpha_{21}|, \delta_{CP})$ plane. Left, middle and right panels show the results for 540 km, 360 km, and 200km baselines, respectively. The light, medium, and dark green contours in each panel correspond to $1\sigma$, $2\sigma$, and $3\sigma$ C.L for 2 degrees of freedom (d.o.f.) i.e., $\Delta \chi^2 = 2.3, 6.18, \text{and } 11.83$ respectively. In this figure we have assumed the standard unitary framework as the true hypothesis, and then we have fitted the non-unitary hypothesis against it. Normal mass ordering has been assumed all over the analyses. The true data have been generated assuming the benchmark choices of the standard unitary oscillation parameters in Table I with $\delta_{CP}(true) = -90^\circ$, while for the reconstruction we have fixed the solar oscillation parameters and marginalized over $\theta_{13}, \theta_{23}, \text{and } \Delta m^2_{31}$. In addition, we have also marginalized over the NU parameters $\alpha_{11}, \alpha_{22}, \text{and } \alpha_{33}$ within their allowed $3\sigma$ ranges as given in Table III. We have also freely varied $\phi_{21}$ from $-\pi$ to $+\pi$. We have assumed zero values of the other non-diagonal NU parameters, $|\alpha_{31}| \text{ and } |\alpha_{32}|$. The red vertical lines in each panel indicate the current $3\sigma$ upper limit on $|\alpha_{21}|$ from neutrino data. One sees that the 200 km baseline gives the best $1\sigma$, $2\sigma$, and $3\sigma$ sensitivities on $|\alpha_{21}|$, in comparison to the 360 km and 540 km baseline option. Quantitatively, the attainable upper limits for $|\alpha_{21}|$ at $1\sigma$ C.L are 0.044, 0.024, and 0.02 for 540 km, 360 km, and 200 km baselines, respectively. Conversely, we have checked that, there is basically no sensitivity to the new CP phase $\phi_{21}$ for any of the baselines. On the other hand, the measurement on $\delta_{CP}$ is not affected much by the presence of non-unitarity. One can also see that
FIG. 3. Upper panels: $\nu_\mu \rightarrow \nu_e$ and $\bar{\nu}_\mu \rightarrow \bar{\nu}_e$ appearance event-spectra as a function of reconstructed neutrino energy at ESSnuSB for different baselines, as indicated. Solid lines represent the standard three-neutrino spectra generated with the standard oscillation parameter values from Table I with $\delta_{\text{CP}} = -90^\circ$ and dashed lines correspond to the NU scenario taking the optimized values of the standard oscillation parameters (not shown explicitly) and the new physics non-unitarity parameters from Table IV. The lower panels represent the absolute difference in the appearance events between the standard unitary (UN) and the NU scenarios divided by the statistical uncertainty in each bin.

The uncertainty on the measurement of $\delta_{\text{CP}}$ is the lowest for 200 km and the highest for 540 km.

| baseline (km) | $\alpha_{11}$ | $\alpha_{22}$ | $\alpha_{33}$ | $\phi_{23}$ | $|\alpha_{31}|$ | $|\alpha_{32}|$ |
|--------------|---------------|---------------|---------------|--------------|----------------|----------------|
| 540          | 0.95          | 0.99          | 0.73          | 155$^\circ$  | 0              | 0              |
| 360          | 0.94          | 0.99          | 0.73          | 140$^\circ$  | 0              | 0              |
| 200          | 0.94          | 0.99          | 0.96          | 75$^\circ$   | 0              | 0              |

TABLE IV. Non-unitarity parameters used for obtaining the non-unitary spectra (dashed line) in Fig. 3, see text for more details.
To understand better the previous result one can select a point allowed at 1, 2, and 3σ for a 540, 360, and 200 km baseline, respectively. We show in Fig. 3 the appearance event spectra for the neutrino (upper-left panel) and antineutrino mode (upper-right panel). For each of the three different baselines we choose a benchmark point (magenta star in Fig. 2) given by the NU parameter $|\alpha_{21}| = 0.04$ and the standard CP phase $\delta_{\text{CP}} = -90^\circ$. For this benchmark choice, the other NU parameters arising from the $\chi^2$ marginalization take the values shown in Table IV. Note that the optimized values of the standard oscillation parameters are not shown here explicitly. We use all of them as input to generate the event spectra in Fig. 3. These are shown as dashed lines, while the unitary scenario is represented with solid lines. In order to better compare the standard unitary (UN) with the NU case, we show in the lower panels of Fig. 3 the absolute differences of the number of events divided by the statistical uncertainty in each bin i.e., $\Delta = |N_{\text{UN}} - N_{\text{NU}}|/\sqrt{N_{\text{UN}}}$. This provides a crude measurement of the statistical significance of our unitarity test. One sees that the best sensitivities to the standard parameter $\delta_{\text{CP}}$ and the NU parameter $|\alpha_{21}|$ are achieved for the 200 km baseline, as already shown in Fig. 2. Notice also that the 360 km baseline does somewhat better than the 540 km baseline. This is also reflected in Fig. 4.

In Fig. 4, we show the one-dimensional projection of the $\Delta \chi^2$ as a function of the absolute value of the NU parameter $|\alpha_{21}|$. As before, this figure is obtained assuming the standard unitary

![Graph showing one-dimensional $\chi^2$ projection on the off-diagonal NU parameter $|\alpha_{21}|$. The red, blue, and green curves represent the allowed boundaries corresponding to three baselines 540 km, 360 km, and 200 km, respectively. Normal mass ordering has been assumed in the analysis, see text.](attachment:image.png)
framework as the true hypothesis, and testing the NU framework against it, i.e. \( \Delta \chi^2 = \chi^2_{\text{NU}} - \chi^2_{\text{UN}} \).

The true values of the oscillation parameters are taken from Table I, fixing the two solar parameters \( \theta_{12} \) and \( \Delta m^2_{21} \) at their benchmark choices, and marginalizing over \( \theta_{13} \), \( \theta_{23} \), and \( \Delta m^2_{31} \). Since the exact value of the standard CP phase \( \delta_{\text{CP}} \) is currently not accurately known, we have marginalized over its true and test values within its full range. Moreover, we have also freely varied the NU parameters \( \phi_{21} \) from \(-\pi\) to \(+\pi\), \( \alpha_{11} \), \( \alpha_{22} \), and \( \alpha_{33} \) within their allowed 3\sigma ranges as given in Table III. We have set the other non-diagonal NU parameters \( |\alpha_{31}| \) and \( |\alpha_{32}| \) to zero. The red, blue, and green curves in the figure indicate the sensitivities to \( |\alpha_{21}| \) for the three baseline choices. As before, the best sensitivity comes from the 200 km baseline, followed by the 360 km and 540 km baselines, respectively. The expected 90% C.L. upper limits corresponding to 540 km, 360 km, and 200 km baselines are 0.08, 0.035 and 0.02, respectively. These limits would be independent and complementary to those given in Table III and constitute a window of opportunity for the ESSnuSB in probing new physics. Notice that the sensitivities expected at ESSnuSB are quite competitive and, for the smaller baselines, it performs better than DUNE [7]. In contrast, the sensitivity of ESSnuSB on \( |\alpha_{31}| \) is very poor, as it does not appear in the vacuum expression of the appearance probability in Eq. 16, and the matter effects in this experiment are rather small.

B. CP violation discovery potential

Now we turn back to the “conventional” CP violation discovery potential within our generalized non-unitary framework. The CP violation (CPV) discovery potential of the ESSnuSB setup is summarized in Fig. 5, for our reference baseline choices. Our results are given both within the unitary as well as in the non-unitary framework. As in the standard \( \delta_{\text{CP}} \) sensitivity study [5], the CP-violating hypothesis is tested against a CP-conserving scenario through [7]

\[
\Delta \chi^2(\delta_{\text{CP}}^{\text{true}}) = \text{Min} \left[ \Delta \chi^2(\delta_{\text{CP}}^{\text{true}}, \delta_{\text{CP}}^{\text{test}} = 0), \Delta \chi^2(\delta_{\text{CP}}^{\text{true}}, \delta_{\text{CP}}^{\text{test}} = \pm \pi) \right].
\]  

This way, we obtain the significance with which one can reject the test hypothesis of no CP violation. The black solid line in each panel corresponds to the standard three-neutrino unitary framework. Upper, middle, and lower panels represent the results obtained for 540 km, 360 km, and 200 km baselines, respectively. The red, green, and blue dashed curves in the left plots represent the CPV discovery sensitivities in the NU framework corresponding to given \( |\alpha_{21}| \) choices, i.e. 0.01, 0.02, and 0.03, respectively (the latter, relatively large value, is taken for comparison). We have assumed five nonzero NU-parameters, which are three diagonal ones, plus one non-diagonal parameter, either \( |\alpha_{21}| \) (left panels) or \( |\alpha_{31}| \) (right panels), with the associated complex CP phase \( (\phi_{21} \text{ or } \phi_{31}) \). In the standard unitary case, we have marginalized over the two mixing angles \( \theta_{13} \) and \( \theta_{23} \) and the mass-squared splitting \( \Delta m^2_{31} \).

In order to perform our unitarity test analysis in the left panels of Fig. 5 we marginalize over the true and test values of the NU parameters \( \alpha_{11}, \alpha_{22}, \alpha_{33}, \text{ and } \phi_{21} \) within their allowed
ranges. One sees that the CPV sensitivity in the standard unitary framework always lies around $8\sigma$ C.L. for $\delta_{CP}(\text{true}) = \pm 90^\circ$ for all three baselines. This agrees with the results presented in Refs. [32, 39, 56]. All baselines have more or less similar sensitivities, except for the fact that the $\delta_{CP}$ range over which CPV can be established for 540 km and 360 km is somewhat bigger than for 200 km. This fact is also confirmed in Ref. [32]. However, we will see the merits of the 200 km baseline in what follows. As far as the NU framework is concerned, two of our benchmark values, $|\alpha_{21}| = 0.01$, and 0.02 lie within the current 3$\sigma$ limit, whereas $|\alpha_{21}| = 0.03$ lies slightly outside the current allowed limit, and could be regarded as a hint for non-unitarity.

We stress that the CPV discovery sensitivity is degraded with respect to the unitary case. This is to be expected, due to the presence of new phases associated to unitarity violation. Clearly, the CPV discovery sensitivity decreases with the increasing $|\alpha_{21}|$ values, specially for 540 km, leading to a minimum $\sim 4.6\sigma$ sensitivity for $\delta_{CP}(\text{true}) = \pm 90^\circ$. The deterioration of the CPV sensitivity is smaller for 360 km and, with a minimum $\sim 5.7\sigma$ sensitivity for $\delta_{CP}(\text{true}) = \pm 90^\circ$. For the 200 km baseline, the deterioration further reduces, with a minimum $\sim 6.1\sigma$ sensitivity for all three benchmark choices, at $\delta_{CP}(\text{true}) = \pm 90^\circ$. All in all one sees that the degrading in CP sensitivity is not as large as one might expect, indicating robustness of the oscillation picture with respect to unitarity violation. The best sensitivities to $\delta_{CP}$ and the non-unitary parameter $|\alpha_{21}|$ are achieved for a 200 km baseline. The results for the 360 km and 540 km baselines can also be seen in Fig. 4.

We now turn to the right panels of Fig. 5. There, we repeated the same analysis for the non-diagonal parameter $|\alpha_{31}|$ and its associated CP phase, $\phi_{31}$. The three benchmark choices considered for $|\alpha_{31}|$ are 0.03, 0.07, and, 0.10. In this case, one finds a mild deterioration of the CPV sensitivity in comparison to the unitary framework for all baselines, so the impact of $|\alpha_{31}|$ is not significant for 540 km, and negligible for 360 km and 200 km baselines. This is attributed to the fact that $|\alpha_{31}|$ does not appear in the vacuum appearance probability, Eq. (16), and also because of the lower matter effects for ESSnuSB with respect to DUNE [7, 57]. As expected, one finds a negligible impact of unitarity violation in this case.

C. CP Reconstruction

In our simplest scenario there are two relevant CP phases, the standard three-neutrino Dirac phase $\delta_{CP}$ and the phase $\phi_{21}$ associated to non-unitarity. One can therefore have four CP conserving cases, when either of them equals 0 or $\pi$. Likewise, four cases in which one has “maximal” CP violation, defined by having the modulus of any of them equal to $\pi/2$. In this section we discuss how well the European spallation source setups can reconstruct the standard CP phase $\delta_{CP}$ as well as the non-unitarity phase $\phi_{21}$ for a few selected benchmarks.

\footnote{Note that $|\alpha_{31}|$ enters only through matter effects, strongly suppressing sensitivity to the associated phase $\phi_{31}$.}

\footnote{The latter would be an indirect manifestation associated to the possible existence of seesaw mediators [8].}
We have fixed $|\alpha_{21}|$ (left panel) and $|\alpha_{31}|$ (right panel) in the data as well as in the theory. We have marginalized over $\theta_{13}, \theta_{23}, \Delta m_{21}^2$, with true and test values of $\alpha_{11}, \alpha_{22}, \alpha_{33}$, and $\phi_{21}$ (in the left panel) and $\phi_{31}$ (in the right panel) within their allowed ranges.
In Fig. 6 we show that assuming different baselines and benchmark parameter values as true. The upper two panels correspond to the two CP conserving cases \((0,0)\) and \((\pi,\pi)\), respectively, while the lower two panels are for the two CP violating scenarios \((-\pi/2,-\pi/2)\) and \((\pi/2,\pi/2)\). The red, green, and cyan contours in each panel correspond to 540 km, 360 km, 200 km baselines of the ESSnuSB experiment, respectively, whereas the orange contours represent the sensitivity expected in DUNE. All contours correspond to the 2\(\sigma\) C.L. for 2 d.o.f. For this analysis, we have fixed \(|\alpha_{21}| = 0.03\), which lies slightly above the current 3\(\sigma\) allowed boundary. All other off-diagonal NU parameters have been kept fixed to zero. We have marginalized over the mixing angles \(\theta_{13}\) and \(\theta_{23}\) and the atmospheric mass-squared splitting, \(\Delta m^2_{31}\). In addition, we have also marginalized over the true and test values of the NU parameters \(\alpha_{11}, \alpha_{22}, \alpha_{33}\) within their allowed ranges.

The expected 1\(\sigma\) uncertainties on \(\delta_{\text{CP}} (\phi_{21})\) for the CP-violating scenarios are 16\(^\circ\) (55\(^\circ\)) for 540 km, 13\(^\circ\) (42\(^\circ\)) for 360 km. On the other hand, for the 200 km baseline, the typical 1\(\sigma\) level uncertainty on \(\delta_{\text{CP}} (\phi_{21})\) is 12\(^\circ\) (22\(^\circ\)). At the 1\(\sigma\) level, the uncertainties on the reconstructed CP phase \(\delta_{\text{CP}} (\phi_{21})\) for our chosen CP conserving benchmarks are 16\(^\circ\) (130\(^\circ\)) for 540 km, 13\(^\circ\) (50\(^\circ\)) for 360 km, as shown in the plots. One sees that the 360 km baseline performs better than 540 km, whereas the best performance could be obtained with 200 km. For comparison, we have also projected the sensitivity of the DUNE experiment in the same plot. For DUNE, the typical 1\(\sigma\) level uncertainty on the reconstructed CP phase \(\delta_{\text{CP}} (\phi_{21})\) is 21\(^\circ\) (35\(^\circ\)).

In short, one can see that the \(\delta_{\text{CP}}\) reconstruction capability of ESSnuSB does not get too much impaired by the presence of unitarity violation, even for a somewhat large value of \(|\alpha_{21}|\). On the other hand, the NU phase determination is competitive with that in DUNE and, in fact, in some cases better.

VI. SUMMARY AND CONCLUSIONS

Here we have explored the physics potential of the proposed European Spallation Source facility in the presence of non-unitarity of the lepton mixing matrix, as generally expected within the seesaw paradigm. First, we have discussed in detail the theoretical framework of neutrino oscillations with effective non-unitary neutrino mixing, discussing in Fig. 1 the resulting neutrino and antineutrino appearance oscillation probabilities. Throughout the paper we have assumed normal neutrino mass ordering, and considered three reference baseline choices of 540 km, 360 km, and 200 km. In Fig. 2 we have presented the sensitivity contours in the \((|\alpha_{21}|, \delta_{\text{CP}})\) plane. The promising results for the 200 km baseline were understood in terms of the expected \(\nu_\mu \rightarrow \nu_e\) and \(\bar{\nu}_\mu \rightarrow \bar{\nu}_e\) appearance event spectra. These are given in Fig. 3 as a function of the reconstructed neutrino energy. We found encouraging ESSnuSB sensitivities for the off-diagonal NU parameter \(|\alpha_{21}|\), as seen in Fig. 4. Perhaps more remarkable is the CPV discovery potential, illustrated in Fig. 5, where one appreciates a relatively mild degrading in sensitivity with respect to the standard unitary
mixing. ESSnuSB would therefore contribute to establishing the robustness of CP determination against small non-unitarity arising, say, from the seesaw mechanism.

We have also obtained a promising CP reconstruction potential, both for the standard CP phase of the three-neutrino paradigm, as well as for the phase associated to non-unitarity, Fig. 6. Altogether, within the generalized non-unitary neutrino mixing framework, we have found that the proposed ESSnuSB facility is competitive and complementary to DUNE, not only for leptonic CP violation studies, but also for probing new physics parameters associated to unitarity violation.
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