Probing CP violation with non-unitary mixing in long-baseline neutrino oscillation experiments: DUNE as a case study

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Abstract

When neutrino masses arise from the exchange of neutral heavy leptons, as in most seesaw schemes, the effective lepton mixing matrix N describing neutrino propagation is non-unitary, hence neutrinos are not exactly orthonormal. New CP violation phases appear in N that could be confused with the standard phase $\delta_{\rm CP}$ characterizing the three neutrino paradigm. We study the potential of the long-baseline neutrino experiment DUNE in probing CP violation induced by the standard CP phase in the presence of non-unitarity. In order to accomplish this we develop our previous formalism, so as to take into account the neutrino interactions with the medium, important in long baseline experiments such as DUNE. We find that the expected CP sensitivity of DUNE is somewhat degraded with respect to that characterizing the standard unitary case. However the effect is weaker than might have been expected thanks mainly to the wide neutrino beam. We also investigate the sensitivity of DUNE to the parameters characterizing non-unitarity. In this case we find that there is no improvement expected with respect to the current situation, unless the near detector setup is revamped.

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I. INTRODUCTION

Following the celebrated discovery of neutrino oscillations [1, 2] subsequent accelerator and reactor studies have brought neutrino physics to the mature phase of precision studies. Sensitive laboratory oscillation studies not only play a key role in confirming the neutrino oscillation hypothesis, but also rule out exotic solutions, establishing the robustness of the simplest three neutrino paradigm.

Given its importance, more than ever it has become relevant to critically assess with improved sensitivity the robustness of the determination of the three-neutrino oscillation parameters within recent and current studies [3–10] as well as future experiments [11]. This includes the scrutiny of the uncertainties associated with neutrino fluxes, propagation and interactions. These may arise, for example, from helioseismology [12, 13], solar chemical composition and solar fusion reactions [14], density fluctuations deep within the Sun [15, 16] as well as magnetic fields in the radiative [17–19] and convective zones [20–23]. On the other hand the subleading role of neutrino non-standard interactions upon oscillations has been considered in various contexts and can also bring new sources of CP violation [24–28]. These issues have been widely explored, so here we focus on the impact of non-unitarity of the lepton mixing matrix upon neutrino propagation and the resulting expected sensitivities on the three–neutrino CP phase determination [29–31].

Non-unitarity of the lepton mixing matrix constitutes a most generic feature of schemes where neutrino masses arise from the exchange of fermionic messengers [32, 33] such as the type-I seesaw mechanism [34–37]. Indeed there is a large class of low-scale variants of the seesaw mechanism, such as inverse and linear seesaw [38–41], where these right-handed neutrino messengers are not-so-heavy, as their masses could lie within reach of the LHC experiments. In this case one expects sizeable departures from unitarity in the lepton mixing matrix characterizing the light neutrino sector [29, 30]. This brings in CP violation associated to the messenger sector into the physics describing the propagation of the light neutrinos [33]. The presence of unitarity violation makes it difficult to extract reliable information on leptonic CP violation and, indeed, first quantitative studies indicate the existence of a potentially serious ambiguity in probing CP violation in neutrino oscillations in such case [31]. As a result, dedicated leptonic CP violation studies taking into account the non-unitarity of the lepton mixing matrix will be necessary. Such studies can shed light on the seesaw scale, and thereby provide valuable insight on the scale of new physics responsible for neutrino mass generation.

In this paper we focus on the possible ambiguities in the CP phase determination for the upcoming DUNE experiment, including matter effects in a consistent way. The paper is organized as follows. In order to set up the framework in section II we compile and update the bounds on the relevant parameters. These follow, for instance, from weak universality tests and short–distance neutrino oscillation searches. In section III we discuss the neutrino effective matter potential in the presence of non-unitarity and present the corresponding results for the oscillation probabilities in matter. In section IV we study the sensitivity of the DUNE experiment to non-unitary neutrino mixing. First we discuss the determination of the standard three-neutrino CP phase $\delta_{\rm CP}$ and the possible confusion with the seesaw phase. Finally we analyze the potential capability of DUNE in further constraining the non-unitarity of the light neutrino mixing matrix. We find that, although the potential to probe CP violation is somewhat degraded with respect to the unitary case, the effect is weaker than expected [31] thanks to the good statistics expected and the relatively wide band neutrino beam at DUNE. Further discussion and conclusions are summarized in section V.

II. PRELIMINARIES: PRIOR CONSTRAINTS

Within a large variety of seesaw schemes the lepton mixing matrix describing the propagation of the light neutrinos is effectively non-unitary, hence these neutrino states are not exactly orthonormal [32]. The description of this situation can be readily obtained by truncating the symmetrical parametrization of the full rectangular lepton mixing matrix characterizing general seesaw schemes, first given in [37]. The resulting form can be written as [30]

$$N = N^{NP} U = \begin{pmatrix} \alpha_{11} & 0 & 0 \\ \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix} U \,, \tag{1}$$

where U is the conventional unitary mixing matrix describing neutrino propagation in the standard case, and the pre-factor parametrizes the deviations from unitarity. This convenient description is general and holds for any number of extra neutrino states [37, 42]. It involves three real parameters α_{11}, α_{22} and α_{33} (all close to one) plus three small complex parameters $\alpha_{21}, \alpha_{31}, \alpha_{32}$ containing extra CP violation. The resulting form provides the most general framework to describe neutrino oscillations relaxing the unitarity approximation.

In order to set the stage for our analysis we first give a brief review on the constraints on non-unitarity parameters. In what follows we update the discussion given in [30, 33], e.g. by including recent results for observables coming from pion decay studies [43]. We also discuss the interplay, as well as the complementarity, of various "prior" restrictions with what can be learned by direct neutrino studies. The bottom-line of our discussion will be that few of these constraints are of general validity, most are model-dependent.

A. Weak interaction without universality: formalism

Here we show how, from general considerations, the constraints from weak no-universality translate into restrictions on non-diagonal α_{ij} parameters. In order to see this, we consider the parametrization of the non-unitary lepton mixing matrix in Eq. 1. The diagonal entries of the pre-factor matrix are given as a product of cosines [30]:

$$\alpha_{11} \;=\; c_{1\,n}\,c_{1\,n-1}c_{1\,n-2}\ldots c_{14}, \tag{2}$$

while the non-diagonal parameters are expressed as [30]:

$$\begin{aligned}\alpha_{21} \;&=\; c_{2\,n}\,c_{2n-1}\ldots c_{2\,5}\,\eta_{24}\bar{\eta}_{14} \;+\; c_{2\,n}\;\ldots c_{2\,6}\,\eta_{25}\bar{\eta}_{15}\,c_{14} \\ &+\;\; \ldots + \eta_{2n}\bar{\eta}_{1n}\,c_{1n-1}\,c_{1n-2}\;\ldots\;c_{14}\end{aligned} \tag{3}$$

with the phase factors $\eta_{ij} = e^{-i\phi_{ij}}\sin\theta_{ij}$ and $\bar{\eta}_{ij} = -e^{i\phi_{ij}}\sin\theta_{ij}$ [37]. Since the "heavy" iso-singlet admixture is assumed to be small, within the framework of seesaw schemes, as well as from experimental evidence [44], we now treat unitarity violation as a perturbation, making use of an small-angle expansion in $\theta_{i\beta}$, with $\beta > 3$, so that

$$\alpha_{11}^2 \;\simeq\; 1 - \sum_{i=4}^{N}\theta_{1\,i}^2\,. \tag{4}$$

On the other hand one can show that

$$\alpha_{21} \;\simeq\; -\theta_{24}\theta_{14}e^{-i(\phi_{24}-\phi_{14})} \;-\; \theta_{25}\theta_{15}e^{-i(\phi_{25}-\phi_{15})}\ldots - \theta_{2n}\theta_{1n}e^{-i(\phi_{2n}-\phi_{1n})} \tag{5}$$

so that

$$\begin{aligned}|\alpha_{21}|^2 \;&\simeq\; |\theta_{24}\theta_{14}e^{-i(\phi_{24}-\phi_{14})} \;+\; \theta_{25}\theta_{15}e^{-i(\phi_{25}-\phi_{15})}\ldots : +\theta_{2n}\theta_{1n}e^{-i(\phi_{2n}-\phi_{1n})}|^2 \\ &\leq\; \sum_{i=4}^{N}|\theta_{2i}\theta_{1i}e^{-i(\phi_{2i}-\phi_{1i})}|^2 \;=\; \sum_{i=4}^{N}\theta_{2i}^2\theta_{1i}^2\end{aligned}$$

Now from the triangle inequality relation one can write

$$\sum_{i=4}^{N}\theta_{2i}^2\theta_{1i}^2 \leq \left(\sum_{i=4}^{N}\theta_{2\,i}^2\right)\left(\sum_{i=4}^{N}\theta_{1\,i}^2\right) \tag{6}$$

which implies the relation

$$|\alpha_{21}| \leq \sqrt{(1-\alpha_{11}^2)(1-\alpha_{22}^2)} \tag{7}$$

and similar relations will hold for α_{31} and α_{32}, namely,

$$\begin{aligned}|\alpha_{31}| \;&\leq\; \sqrt{(1-\alpha_{11}^2)(1-\alpha_{33}^2)} \\ |\alpha_{32}| \;&\leq\; \sqrt{(1-\alpha_{22}^2)(1-\alpha_{33}^2)}\end{aligned} \tag{8}$$

One sees that in the limit of small heavy singlet messenger admixture one has,

$$\alpha_{ii} \sim 1 \quad \text{and} \quad \alpha_{ij} \ll 1.$$

These relations imply additional restrictions on non-diagonal entries coming from constraints on the diagonal ones. In the next section we will see that bounds on diagonal entries are relatively strong reinforcing the bounds on non-diagonal ones. This also implies that lepton flavour violation and CP violation rates in the charged sector are constrained mainly by universality restrictions, not by the smallness of neutrino masses themselves. This important observation has previously been made in a number of papers and reviews [45–47]. In the next subsection we compile bounds from universality as well as from the relevant neutrino oscillation experiments.

B. Universality constraints

The non-unitarity of the light neutrino mixing matrix can be constrained by several observables related to weak universality.

- **CKM unitarity**

  As has been widely discussed in the literature [48–56], the comparison of measurements of muon and beta decay rates can constrain the non-unitarity of the neutrino mixing matrix. For example, the Fermi constant value for muon and beta decay will be proportional to different non-unitary parameter combinations:

$$G_\mu = G_F \sqrt{(NN^\dagger)_{11}(NN^\dagger)_{22}} = G_F \sqrt{\alpha_{11}^2(\alpha_{22}^2 + |\alpha_{21}|^2)}, \tag{9}$$

  and

$$G_\beta = G_F \sqrt{(NN^\dagger)_{11}} = G_F \sqrt{\alpha_{11}^2}. \tag{10}$$

  This will imply that the CKM elements V_{ud} and V_{us}, proportional to the Fermi constant G_μ, should be corrected by the corresponding factor and expressed as [49–51]:

$$\sum_{i=1}^{3} |V_{ui}|^2 = \left(\frac{G_\beta}{G_\mu}\right)^2 = \left(\frac{G_F\sqrt{(NN^\dagger)_{11}}}{G_F\sqrt{(NN^\dagger)_{11}(NN^\dagger)_{22}}}\right)^2 = \frac{1}{(NN^\dagger)_{22}}, \tag{11}$$

  The experimental value of this expression is given by [57]:

$$\sum_{i=1}^{3} |V_{ui}|^2 = \frac{1}{\alpha_{22}^2 + |\alpha_{21}|^2} = 0.9999 \pm 0.0006, \tag{12}$$

- **W mass measurements**

  The mass of the W boson, M_W, is related with the values of the weak mixing angle, s_W, and the Fermi constant. Including radiative corrections, in the On-Shell renormalization scheme, this relation can be written as [57]:

$$M_W = \frac{A_0}{s_W(1-\Delta r)^{1/2}}\,, \tag{13}$$

with

$$A_0 = \left(\frac{\pi\alpha}{\sqrt{2}G_F}\right)^{1/2}, \tag{14}$$

$$s_W^2 = 0.22336 \pm 0.00010\,, \tag{15}$$

$$\Delta r = 0.03648 \pm 0.00031\,, \tag{16}$$

where Δr includes the radiative corrections relating α, $\alpha(M_Z)$, G_F, M_W and M_Z. In the non-unitary case, the Fermi constant should take into account the corresponding corrections and the prescription for A_0 will be:

$$A_0 = \left(\frac{\pi\,\alpha\,\sqrt{\alpha_{11}^2(\alpha_{22}^2+|\alpha_{21}^2|)}}{\sqrt{2}G_\mu}\right)^{1/2}. \tag{17}$$

- **semileptonic weak decays**

  The couplings between leptons and gauge bosons are dictated by gauge symmetry. For the standard case of lepton unitarity these are flavor independent. This feature is no longer true in the presence of non-unitarity. As a result, the ratio between two different semileptonic decay rates would constrain non-unitarity parameters. For example, for the case of pion decay we have [52]:

$$R_\pi = \frac{\Gamma(\pi^+ \to e^+\nu)}{\Gamma(\pi^+ \to \mu^+\nu)} = \frac{(NN^\dagger)_{11}}{(NN^\dagger)_{22}} = \frac{\alpha_{11}^2}{\alpha_{22}^2+|\alpha_{21}|^2}. \tag{18}$$

  Here we include the updated measurement from Ref. [43] and theoretical prediction in Refs. [58, 59]:

$$r_\pi = \frac{R_\pi}{R_\pi^{SM}} = \frac{(1.2344 \pm 0.0029)\times 10^{-4}}{(1.2352 \pm 0.0002)\times 10^{-4}} = 0.9994 \pm 0.0030. \tag{19}$$

  Notice that this constraint is more restrictive than the previously reported value, $r_\pi = 0.9956 \pm 0.0040$ [60]. One also has the corresponding bound from Kaon-decay [52]

$$r_K = \frac{R_K}{R_K^{SM}} = \frac{(NN^\dagger)_{11}}{(NN^\dagger)_{22}} = \frac{\alpha_{11}^2}{\alpha_{22}^2+|\alpha_{21}|^2} = \frac{(2.488 \pm 0.010)\times 10^{-5}}{(2.477 \pm 0.001)\times 10^{-5}} = 1.004 \pm 0.010. \tag{20}$$

  However, this limit does not play a significant role, since the pion decay measurements are more restrictive.

- **$\mu - \tau$ universality**

  Likewise, for the case of $\mu - \tau$ universality there are restrictions that follow from the ratio of the decay of the meson (π^- or K^-) to a muon plus a muon neutrino, or from the tau decay to a meson and a tau neutrino [30, 51, 61]:

$$R_{\tau/P} = \frac{\Gamma(\tau^- \to P^- \nu_\tau)}{\Gamma(P^- \to \mu^+ \nu_\mu)} \propto \left| \frac{g_\tau}{g_\mu} \right|^2 = \frac{\alpha_{33}^2 + |\alpha_{32}|^2 + |\alpha_{31}|^2}{\alpha_{22}^2 + |\alpha_{21}|^2}, \tag{21}$$

where P^- stands for either π^- or K^- mesons. Several ratios can be considered and included in the analysis. In particular we have considered the results reported in Ref. [61].

- $e - \tau$ **universality**

  On the other hand, for the e - τ sector, we have considered only pure leptonic decays as well as direct leptonic decays of W boson, which lead to

$$\left| \frac{g_e}{g_\tau} \right|^2 = \frac{\alpha_{11}^2}{\alpha_{33}^2 + |\alpha_{32}|^2 + |\alpha_{31}|^2} \,. \tag{22}$$

  The value of $|g_e/g_\tau|$ ratio for each process was presented in Ref. [61].

- Invisible Z decay width

  Non-unitarity can affect the neutral current couplings. As noted in [37], these are no longer "trivial" as in the standard model since the couplings of light neutrinos to the Z-boson can be non-diagonal in the mass basis. Moreover the diagonal coupling strengths are smaller than in the standard model thereby decreasing the invisible Z width, well measured at LEP and reported to be slightly smaller than three (2.9840 ± 0.0082) [62]. However, neutral currents have a more complex structure that will depend both on the values of the α parameters as well as on the values of the three by three matrix $U^{3\times3}$. Given this complexity and the quadratic dependence on the α, it is safe not to include this observable into the analysis.

Concerning searches for lepton flavor and CP violating processes we notice that these do not give us any independent robust constraint on unitarity violation. Indeed, such processes may proceed in the absence of neutrino mass and are only restricted by weak universality tests [45, 47, 63].

C. Neutrino oscillation constraints

Direct constraints on the non-diagonal elements of the N matrix come from the so-called zero distance effect in the conversion probability [32]. For example, the conversion probability from muon to electron neutrinos can be written as [30],

$$P_{\mu e} \simeq (\alpha_{11}\alpha_{22})^2 P_{\mu e}^{3\times3} + \alpha_{11}^2\alpha_{22}|\alpha_{21}|P_{\mu e}^I + \alpha_{11}^2|\alpha_{21}|^2, \tag{23}$$

	One parameter (1 d.o.f.)		All parameters (6 d.o.f.)	
	90% C.L.	3σ	90% C.L.	3σ
Neutrinos + charged leptons				
$\alpha_{11} >$	0.9974	0.9963	0.9961	0.9952
$\alpha_{22} >$	0.9994	0.9991	0.9990	0.9987
$\alpha_{33} >$	0.9988	0.9976	0.9973	0.9961
$\|\alpha_{21}\| <$	1.7×10^{-3}	2.5×10^{-3}	2.6×10^{-3}	4.0×10^{-3}
$\|\alpha_{31}\| <$	2.0×10^{-3}	4.4×10^{-3}	5.0×10^{-3}	7.0×10^{-3}
$\|\alpha_{32}\| <$	1.1×10^{-3}	2.0×10^{-3}	2.4×10^{-3}	3.4×10^{-3}
Neutrinos only				
$\alpha_{11} >$	0.98	0.95	0.96	0.93
$\alpha_{22} >$	0.99	0.96	0.97	0.95
$\alpha_{33} >$	0.93	0.76	0.79	0.61
$\|\alpha_{21}\| <$	1.0×10^{-2}	2.6×10^{-2}	2.4×10^{-2}	3.6×10^{-2}
$\|\alpha_{31}\| <$	4.2×10^{-2}	9.8×10^{-2}	9.0×10^{-2}	1.3×10^{-1}
$\|\alpha_{32}\| <$	9.8×10^{-3}	1.7×10^{-2}	1.6×10^{-2}	2.1×10^{-2}

TABLE I: Bounds on the magnitudes of the non-unitarity parameters at 90% C.L. and 3σ (for 1 and 6 d.o.f.). Upper table: constraints coming from neutrinos and charged leptons. Lower part: constraints derived from direct neutrino oscillation searches [44, 64, 65].

after neglecting cubic products of the small parameters α_{21}, $\sin\theta_{13}$ and Δm^2_{21}. Here, $P^{3\times3}_{\mu e}$ stands for the standard conversion probability in the unitary case, while the interference probability term $P^{I}_{\mu e}$ depends on the non-unitarity parameters, including an additional CP phase. Finally, the last term in this expression is a constant factor, independent of the distance travelled by the neutrino and its energy. Therefore, any neutrino appearance experiment in the $\nu_\mu \to \nu_e$ channel would be sensitive to this zero distance (0d) contribution:

$$P^{0d}_{\mu e} = \alpha^2_{11}|\alpha_{21}|^2. \tag{24}$$

There is a similar expression for the conversion probability in the $\nu_e \to \nu_\tau$ and $\nu_\mu \to \nu_\tau$ channels. In the latter case, the oscillation probability formula is slightly more complicated, but at leading order in the non-unitary parameters, one can approximate both zero-distance appearance probabilities by

$$P^{0d}_{e\tau} = \alpha^2_{11}|\alpha_{31}|^2\,, \tag{25}$$

$$P^{0d}_{\mu\tau} \simeq \alpha^2_{22}|\alpha_{32}|^2\,. \tag{26}$$

We have used these expressions to obtain direct constraints on the parameters $|\alpha_{21}|$, $|\alpha_{31}|$ and $|\alpha_{32}|$ using the negative searches from the NOMAD and CHORUS short-baseline experiments. NOMAD [44, 65] reported limits on the search for $\nu_\mu \to \nu_e$ as well as $\nu_\mu \to \nu_\tau$ oscillations in a predominantly ν_μ neutrino beam produced by the SPS at CERN, while CHORUS [66, 67] used the same beam to search for $\nu_\mu \to \nu_\tau$ oscillations. Additionally, from the contamination of electron neutrinos in the beam, they were also able to constrain the oscillation channel $\nu_e \to \nu_\tau$. The stronger bounds at 90% C.L. from these experiments, obtained by NOMAD, can be summarized as:

$$\begin{aligned} P^{0d}_{\mu e} &< 7.0 \times 10^{-4} \\ P^{0d}_{\mu\tau} &< 1.6 \times 10^{-4} \\ P^{0d}_{e\tau} &< 0.74 \times 10^{-2} \end{aligned} \tag{27}$$

Similar constraints can also be obtained from the NuTeV data [68]. Note that, in addition to the short-baseline experiments discussed above, there are also nontrivial constraints arising from medium and long-baseline experiments in combination with atmospheric and solar neutrino data [64, 69]. For maximal values of the diagonal parameters α_{ii}, one can summarize the bounds obtained in [64] in terms of 3σ limits on the non-diagonal parameters:

$$\begin{aligned} |\alpha_{21}| &< 0.03 \\ |\alpha_{31}| &< 0.11 \\ |\alpha_{32}| &< 0.12 \end{aligned} \tag{28}$$

We stress that the above constraints coming from neutrino oscillations are independent of the mass scale of the heavy neutrinos. Therefore, they can be used to constrain the non-unitarity of the lepton-mixing matrix independent on the heavy mass scale. These are the only fully model-independent constraints. Therefore, such neutrino-data-only bounds play a special role and for this reason have been separated as the lower part in Table I. This Table summarizes all the available non-unitarity bounds discussed in this section. Clearly, as seen from the upper part of Table I, one can see that universality tests provide strong constraints on the diagonal parameters, α_{ii}, that are very close to unity, independently of the number of degrees of freedom considered. In addition, one can also combine with the relations in Eqs. (7) and (8) in order to obtain stronger constraints on the non-diagonal α parameters. Indeed, by combining universality bounds with these relations one finds that the constraints on the non-diagonal parameters are of order 10^{-3}.

However we note that these limits are all derived from charged current induced processes under the restrictive assumption that there is no new physics other than that of non-unitary mixing. As an example, we note that the presence of neutrino-scalar Yukawa interactions, absent in the standard model but present in models with extra Higgs bosons, such as multi-Higgs schemes (e.g. incorporating flavor symmetries), would potentially avoid these bounds. Likewise, the presence of right-handed charged current contributions expected within a left-right symmetric seesaw scheme would have the same effect. This happens if the extra scalar or vector-mediated contributions compensate the unitarity violation effect [1]. Of course one may go beyond the above well-motivated assumptions and consider, for the sake of generality, the most general Lorentz structure for the charged weak interactions [2]. In such case these limits would be invalidated, leading us to regard them as fragile. In contrast, the constraints from neutrino experiments provide a direct restriction on the non-unitarity α parameters. These bounds are significantly less stringent, of the order of 10^{-2} for the non-diagonal α_{ij}, and correspond to the lower entries in Table I.

Finally, there are also direct bounds from searches for neutral heavy leptons. These depend on the mass of the heavy neutrinos, and do not apply beyond the kinematical reach of the high energy experiments, such as LEP [72–74] and LHC [75]. All mass-dependent limits on light and heavy singlet neutrinos have been compiled in Refs. [30, 33, 76–78].

In short, at this stage one may adopt two approaches:

- to use as reference the more restrictive bounds coming from charged current weak processes (upper part of Table I)
- to use as benchmarks bounds taken strictly from the neutrino sector (lower part of Table I).

While the top limits on the α's are stronger, they are not robust enough for our purposes, so we would recommend to focus on the most direct constraints coming from the bottom part of Table I). In any case in our simulations for the DUNE experiment in order to evaluate its potential in probing leptonic CP violation in the presence of unitarity violation we include as benchmark values not only the conservative, but also the model-dependent bounds, for comparison. The bottom-line is that the DUNE experiment will have the potential of providing independent and robust probes of neutrino properties beyond standard oscillations, properties which can not be probed otherwise in a model-independent way.

III. NON-UNITARY OSCILLATION PROBABILITIES IN MATTER

In [30, 31] we have given the analytic expressions for the neutrino oscillation probabilities in vacuum [3]. This approach is valid to study oscillation experiments where matter effects are not very relevant. However, in order to obtain direct sensitivities on the non-unitarity of the lepton mixing matrix from upcoming long-baseline neutrino oscillation experiments such as DUNE or NOνA, one must have a consistent way to describe matter effects appropriate to this situation. In order to quantify the impact of non-unitary mixing in such experiments,

[1] While direct search bounds for such charged mediators are rather stringent, one can still find “fine-tuned” funnels in parameter space which allow the situation envisaged here.
[2] Such model-independent studies of the charged current weak interactions were given in [70, 71].
[3] See Refs. [79, 80], where a different form for the non-unitary neutrino mixing matrix is used.

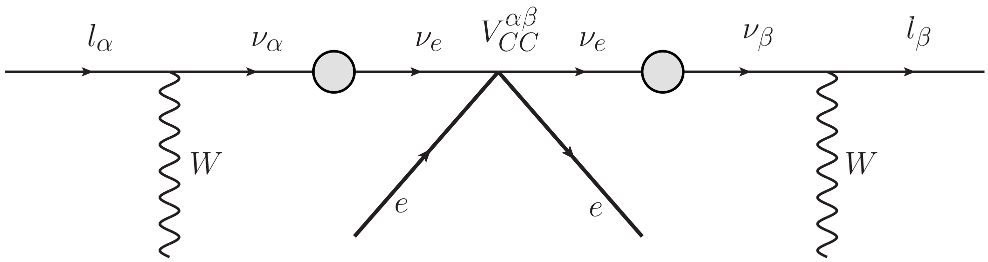

FIG. 1: Feynman diagram illustrating the matter potential associated to the charged current [81].

where matter effects are expected to play an important role, one should take into account how the effective matter potential for neutrinos gets modified in the presence of non-unitary three-neutrino mixing. We discuss this issue in the next subsection.

A. Neutrino effective matter potential in the presence of non-unitarity

The standard derivation of the effective potential that neutrinos feel when traversing a material medium assumes unitary mixing between the light neutrino species [4]. In order to derive the neutrino potential in matter for a model with neutral heavy leptons, we note that the complete expression for the neutrino in a flavor state will be given by

$$\nu_\alpha = \sum_i^n K_{\alpha i}\nu_i \,, \tag{29}$$

with the α subscript indicating flavor and i mass eigenstates. Charged current matter effects in neutrino propagation are illustrated in the Feynman-like diagram in Fig. (1) and will be proportional to

$$K_{\alpha i}K^*_{ei}K_{ej}K^*_{\beta j} = (KK^\dagger)_{\alpha e}\,(KK^\dagger)_{e\beta} \,. \tag{30}$$

Therefore, the charged current potential will be given by

$$V_{CC}^{\alpha\beta} = \sqrt{2}\,G_F N_e \left(KK^\dagger\right)_{\alpha e}\left(KK^\dagger\right)_{e\beta} \,. \tag{31}$$

where N_e is the number density of electrons in the medium and G_F is the Fermi constant. However, the heavy states will not take part in a long baseline neutrino oscillation set up. As a result the sum in Eq. (29) must be performed only up to the third mass eigenstate. Therefore, effectively, one has:

$$\nu_\alpha = \sum_i^3 K_{\alpha i}\nu_i = \sum_i^3 N_{\alpha i}\nu_i \,, \tag{32}$$

[4] We will assume a non-polarized neutral medium in the calculation of the effective matter potential

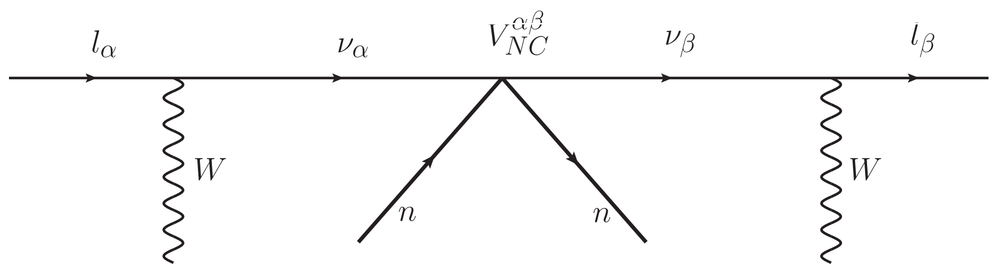

FIG. 2: Feynman diagram illustrating the matter potential associated to the neutral current [32].

and the effective CC potential in the presence of non-unitarity will be given by:

$$V_{CC}^{\alpha\beta} = \sqrt{2}\, G_F N_e \left(NN^\dagger\right)_{\alpha e} \left(NN^\dagger\right)_{e\beta} \; . \tag{33}$$

which is expressed in terms of the α parameters as:

$$(NN^\dagger)_{\alpha e}(NN^\dagger)_{e\beta} = \alpha_{11}^2 \begin{pmatrix} \alpha_{11}^2 & \alpha_{11}\alpha_{21}^* & \alpha_{11}\alpha_{31}^* \\ \alpha_{11}\alpha_{21} & |\alpha_{21}|^2 & \alpha_{21}\alpha_{31}^* \\ \alpha_{11}\alpha_{31} & \alpha_{21}^*\alpha_{31} & |\alpha_{31}|^2 \end{pmatrix} \; . \tag{34}$$

Clearly in the unitary limit ($\alpha_{ii} = 1$ and $\alpha_{ij} = 0$), one recovers the well-known Wolfenstein form for the effective CC potential:

$$V_{CC}^{\alpha\beta} = \sqrt{2} G_F N_e \delta_{\alpha e}\delta_{\beta e} \tag{35}$$

For the neutral current case we proceed in a similar way. Again we consider the Feynman-like diagram of the NC process as described in Fig. 2 and the neutral current potential is given by

$$V_{NC}^{\alpha\beta} = -\sum_\rho \frac{1}{\sqrt{2}} G_F N_n \left(KK^\dagger\right)_{\alpha\rho} \left(KK^\dagger\right)_{\rho\beta} \; . \tag{36}$$

After truncating the rectangular K matrix into the square matrix N, we obtain that the NC contribution to the matter potential is given by:

$$V_{NC}^{\alpha\beta} = -\sqrt{2} G_F \frac{N_n}{2} \sum_\rho (NN^\dagger)_{\alpha\rho}(NN^\dagger)_{\rho\beta} = -\sqrt{2} G_F \frac{N_n}{2} \left[(NN^\dagger)^2\right]_{\alpha\beta} \; , \tag{37}$$

where the matrix product $(NN^\dagger)^2$ at leading order in the non-diagonal α's is given by:

$$\begin{pmatrix} \alpha_{11}^4 & \alpha_{11}\alpha_{21}^* \left(\alpha_{11}^2 + \alpha_{22}^2\right) & \alpha_{11}\alpha_{31}^* \left(\alpha_{11}^2 + \alpha_{33}^2\right) \\ \alpha_{11}\alpha_{21} \left(\alpha_{11}^2 + \alpha_{22}^2\right) & \alpha_{22}^4 & \alpha_{22}\alpha_{32}^* \left(\alpha_{22}^2 + \alpha_{33}^2\right) \\ \alpha_{11}\alpha_{31} \left(\alpha_{11}^2 + \alpha_{33}^2\right) & \alpha_{22}\alpha_{32} \left(\alpha_{22}^2 + \alpha_{33}^2\right) & \alpha_{33}^4 \end{pmatrix} \tag{38}$$

So, one sees how, starting with diagonal CC and NC potentials, due to the non-unitarity one ends up in general with non-diagonal forms for the effective matter potentials.

Notice that the non-unitarity parameters α_{31}, α_{32} and α_{33}, which do not enter in the expression of $P_{\mu e}$ in vacuum [30, 33], do appear in the calculation of $P_{\mu e}$ in matter due to the form of the effective matter potential. The effect of the non-diagonal parameters α_{31} and α_{32} is not as important as the role of α_{21}. The α_{31} parameter enters linearly in the CC and NC potential in the 13 entry. Its effect will be analogous to that of the parameter $\epsilon_{e\tau}$ in the case of non-standard interactions, so that the resulting degeneracy with the reactor angle θ_{13} [82, 83] will imply a deterioration of the sensitivity to CP violation [28]. In contrast, α_{32} will enter only in the neutral current potential in the 23 entry and, therefore, is expected to have a negligible impact.

Adding the two contributions to the effective potential in matter we will have [5]:

$$V^{\alpha\beta} = V_{CC}^{\alpha\beta} + V_{NC}^{\alpha\beta} = \sqrt{2}\, G_F N_e \left(NN^\dagger\right)_{\alpha e} \left(NN^\dagger\right)_{e\beta} - \sqrt{2} G_F \frac{N_n}{2} \sum_\rho (NN^\dagger)_{\alpha\rho} (NN^\dagger)_{\rho\beta} \quad (39)$$

where α and β stands for the initial and final neutrino flavor, respectively, and ρ implies a sum over the three active flavors. N_e is the electron density in the medium while N_n is the neutron density. In matrix form one has the following expression for the matter potential in the presence of non-unitarity:

$$V_{NU} = \left(NN^\dagger\right) \left[\sqrt{2}\, G_F N_e \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \frac{\sqrt{2}}{2}\, G_F N_n \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right] \left(NN^\dagger\right) \quad (40)$$

leading to a very simple compact form

$$V_{NU} = \left(NN^\dagger\right) V_{\text{unitary}} (NN^\dagger) \; . \quad (41)$$

Notice that, in contrast to the standard procedure used in the three–neutrino unitary case, the contribution of the neutral current potential can no longer be neglected when treating the non-unitary case.

One can also see how to get this result from the truncation of the $N \times N$ mixing matrix, U. Therefore, the Hamiltonian in matter in the flavour basis will be given by:

$$H_{NU} = N \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{\Delta m_{21}^2}{2E} & 0 \\ 0 & 0 & \frac{\Delta m_{31}^2}{2E} \end{pmatrix} N^\dagger + \left(NN^\dagger\right) \begin{pmatrix} V_{cc} + V_{nc} & 0 & 0 \\ 0 & V_{nc} & 0 \\ 0 & 0 & V_{nc} \end{pmatrix} \left(NN^\dagger\right) \quad (42)$$

with $V_{cc} = \sqrt{2} G_F N_e$ and $V_{nc} = -\frac{\sqrt{2}}{2} G_F N_n$.

[5] Similar results have been obtained in Ref.[84]

IV. NON-UNITARY NEUTRINO MIXING IN DUNE

Here we explore the expected sensitivities to the non-unitarity of the neutrino mixing matrix within the upcoming DUNE experiment. Previous studies have already considered the impact of non-unitarity upon the CP-phase sensitivity at T2K [85]. Here we present a dedicated study for the DUNE experiment, whose longer baseline implies that matter effects are more relevant than for the cases of T2K and NOvA and therefore the formalism described above is crucial.

A. DUNE simulation with non-unitary neutrino mixing

DUNE is a long-baseline neutrino oscillation experiment that will measure neutrino oscillations over a broad energy range, from hundreds of MeV to few tenths of GeV. This experiment will detect neutrinos and anti-neutrinos produced in the NuMI beam line at Fermilab 1300 km away from the source, with relevant matter effects in the neutrino propagation. The effect of non-unitary neutrino mixing in the DUNE simulation will modify the standard calculation of neutrino oscillation probabilities. Besides the non-unitary neutrino mixing matrix, to calculate the neutrino conversion probability in DUNE one must take into account the modified matter potential affecting neutrino propagation through the Earth, as discussed in the previous section. Using the neutrino Hamiltonian with matter effects as given by Eq. (42), we have solved numerically the evolution equation, obtaining the corresponding conversion probability from muon to electron neutrino in the case of DUNE. We illustrate the behavior of the modified neutrino appearance probability $P_{\mu e}$ for the DUNE experiment in Fig. 3. The left panel corresponds to neutrino probability and the right panel to antineutrino probability. Each band corresponds to a different value of the standard CP phase, $\delta_{\rm CP}$, while the width of the band is due to the variation over the non-unitary phase $\phi_{21} = Arg(\alpha_{21})$. The only deviation from unitarity in this calculation comes from the α_{21} parameter, set to 0.02. The overlap of the different bands indicates the presence of degeneracies in the neutrino oscillation probability in DUNE. This ambiguity, present at the probability level has already been noticed in Ref. [31, 33]

The DUNE experimental setup assumed for this analysis corresponds to a 40–ton liquid argon far detector with optimized neutrino fluxes, cross sections, detector efficiency and energy resolution effects as provided in the form of GLoBES [86, 87] files in Ref. [88]. The calculation of the neutrino oscillation probabilities in the presence of non-unitarity has been implemented in the GLoBES package with an adequate modification of its probability engine. In our analysis, we have used the spectral event information from the four neutrino oscillation channels: electron (anti)neutrino appearance and muon (anti)neutrino disappearance. To statistically quantify the effect of the non-unitary lepton mixing parameters we have used the usual χ^2 definition adding penalties on the 'unitary' oscillation parameters θ_{ij} and Δm^2_{k1} [89].

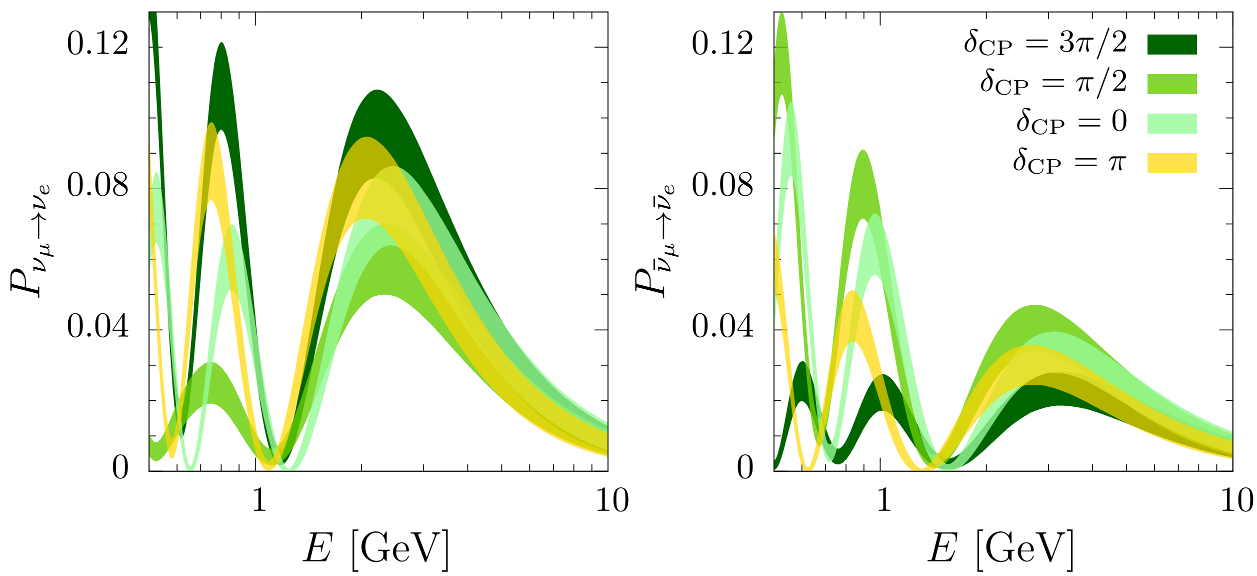

FIG. 3: Neutrino electron appearance probability in DUNE for the neutrino (left) and antineutrino (right panel) channel, with $|\alpha_{21}| = 0.02$ and ϕ_{21} free for fixed value of δ_{CP}.

The relative error on these parameters and the systematic uncertainties in the normalization of signal and background for each oscillation channel, ranging from 0.2% to 20% depending on the channel, were set to the values given in Ref. [88].

For the rest of this section we denote the three mixing angles collectively as a vector $\vec{\lambda} = \{\theta_{ij}, \Delta m^2_{k1}\}$. We have included penalties to the χ^2 accounting for the allowed values of the $\vec{\lambda}$ parameters. Likewise, we denote the non-unitarity parameters in a compact form as $\vec{\alpha} = \{\alpha_{ii}, \alpha_{ij}\}$, including both their diagonal and non-diagonal components. Note that we treat the CP phase δ_{CP} separately.

B. DUNE sensitivity to CP violation

In this section we analyze how DUNE sensitivity to the standard CP violation is affected by the presence of non-unitarity. To the oscillation parameters present in the standard unitary scenario this analysis implies the addition of nine real parameters describing the non-unitary mixing: the three real α_{ii} plus the three complex non-diagonal α_{ij}.

In order to simplify the analysis, we consider however only five non-zero non-unitary parameters at a time: the three diagonal ones, plus one of the non-diagonal ones, with its complex phase at a time. The resulting CP sensitivity in the presence of non-unitarity is shown in Fig. 4. As in the standard $\delta_{\rm CP}$-sensitivity plot, the CP-violation hypothesis is tested with respect to a CP-conserving scenario [11]:

$$\Delta\chi^2(\delta_{\rm CP}^{\rm true}) = {\rm Min}\left[\Delta\chi^2_{CP}(\delta_{\rm CP}^{\rm true}, \delta_{\rm CP}^{\rm test} = 0), \Delta\chi^2_{CP}(\delta_{\rm CP}^{\rm true}, \delta_{\rm CP}^{\rm test} = \pi)\right], \tag{43}$$

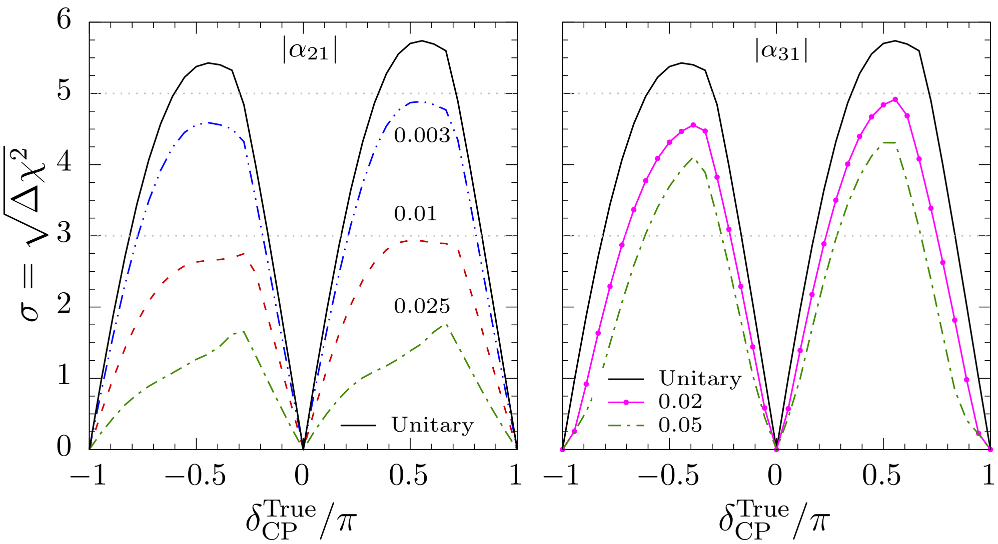

FIG. 4: DUNE sensitivity to CP violation for non-unitary neutrino mixing. For comparison the black solid line shows the CP-sensitivity in DUNE, for the standard unitary case. The reduced sensitivities for non-zero α_{21} (α_{31}) are shown in the left (right) panel. All undisplayed parameters have been marginalized over, including the non-unitarity phases as well as the diagonal parameters α_{ii}.

The remaining standard $\vec{\lambda}$ as well as the non-unitarity parameters $\vec{\alpha} \equiv \{\alpha_{ii}, \phi_{ij}\}$, which are included in both the simulated and reconstructed event rates in DUNE, $n(\vec{\lambda}, \delta_{\rm CP}; \vec{\alpha})$, have been marginalized over. The left panel has been obtained for different values of $|\alpha_{21}|$, while the right panel corresponds to the results of the corresponding analysis performed for the non-diagonal non-unitarity parameter α_{31}. One sees from the left panel that the sensitivity to the Dirac CP phase decreases in the presence of non-unitarity with respect to the standard 'unitary' case, shown in the black-solid line. The remaining lines correspond to the non-unitary case with different values for the α_{21} parameter, as indicated. We have selected three different benchmark values, the smaller one, 0.003, consistent with the upper part of Table I and 0.010 and 0.025 consistent with sensitivities displayed in the lower part of the table, obtained from neutrino data only. Even taking at face value the "aggressive" sensitivity $|\alpha_{21}| = 0.003$, the significance of a CP-violation measurement decreases by 0.85σ, compromising the possibility of testing any range of values of the CP phase at 5σ. For more conservative and reasonable choices $|\alpha_{21}|$ at the 1% level one sees that the presence of non-unitarity precludes our ability to probe CP violation at 3σ for nearly all of the δ_{CP} range. One sees that probing maximal CP violating values $\pm\pi/2$ with high significance in the presence of non-unitarity for 'large' $|\alpha_{21}|$ constitutes a big challenge for DUNE. In the right panel, we show the results of the same analysis for the non-diagonal parameter α_{31}. As we discussed before, the impact of this parameter on the neutrino oscillation probabilities in DUNE is significantly less relevant in comparison with α_{21}. As a result, one can see from the figure that even if the fraction of CP at 5σ is largely reduced respect to the unitary case, the reduction in the significance of CP tests is much smaller than for $|\alpha_{21}|$. This result holds for relatively large values of the parameter compatible with the bounds in the lower part of Table I, namely $|\alpha_{31}| = 0.05$. The effect of the third non-diagonal parameter, α_{32}, is not displayed in the figure. We have checked that it plays nearly no role in the analysis, which confirms our discussion in Section III.

Here we note that Ref. [90] has also discussed the possibility of probing CP violation with T2K, NOvA and DUNE in the presence of non-unitarity. Although we have a qualitative agreement in the loss of CP-sensitivity due to the presence of non-unitarity, our results show some quantitative differences. We ascribe these discrepancies to the treatment of the DUNE simulation. Here we are using the official description released by the DUNE Collaboration, and we have validated our method against the official DUNE CP-sensitivity result for the standard (unitary) oscillation analysis.

C. DUNE sensitivity to non-unitary neutrino mixing

In this section we analyze the potential of DUNE in constraining the non-unitarity of the neutrino mixing matrix. As we have discussed in Section II, the most robust and direct of these constraints come from neutrino oscillation experiments and are not very strong. Therefore, we wish to explore the capability of DUNE in further constraining non-unitarity. For this purpose we will focus in the analysis of the neutrino signal at the DUNE far detector. The capability of the near detector will be analyzed in the future. As we have discussed in the previous subsection, the parameter with the most impact on the DUNE sensitivity to CP violation is α_{21}. As a result we will focus on α_{21} as the key parameter to be constrained in order to characterize the loss of sensitivity in CP searches at DUNE. Following the usual procedure in analyzing the sensitivity of a given experiment to an unknown parameter (the non-unitary parameter α_{21} in this case), we have simulated DUNE events under the hypothesis of unitary mixing $n^{\text{true}}(\vec{\lambda}, \delta_{\text{CP}}^{\text{true}})$. Afterwards, we have tried to reconstruct DUNE data in terms of the non-unitary neutrino mixing ansatz, $n^{\text{test}}(\vec{\lambda}, \delta_{\text{CP}}^{\text{test}}; \vec{\alpha})$. It is worth noticing that the treatment of the non-unitarity here is different from the analysis performed in the previous subsection and therefore a direct comparison between the results presented in Figs. 4 and 5 is not straightforward. For this analysis, the true value of the Dirac CP phase has been fixed to its current preferred value, $\delta_{\text{CP}}^{\text{True}} = -\pi/2$. After marginalizing over the diagonal non-unitary parameters and all the oscillation parameters but δ_{CP}, we obtained the allowed parameter regions (at $1-4\sigma$ for 2 d.o.f) shown in Fig. 5. In the left panel, the allowed regions in the $\delta_{\text{CP}} - |\alpha_{21}|$ plane show that DUNE is sensitive to values of $|\alpha_{21}|$ at the percent level at 1σ. As expected, the best fit point for the Dirac CP phase is equal to the assumed 'true' value. However, for large enough values of $|\alpha_{21}|$, degenerate solutions around $\delta_{\text{CP}} = \pm\pi$ appear at higher C.L.

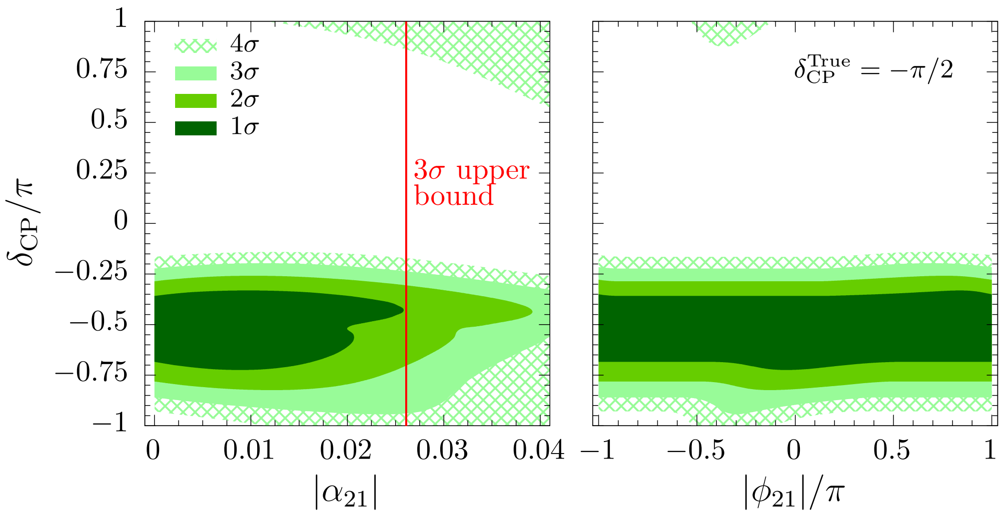

FIG. 5: Testing non-unitary neutrino mixing against the standard case, when only the off–diagonal parameter α_{21} is present. In the left (right) panel, the α_{21}–δ_{CP} (ϕ_{21}–δ_{CP}) allowed parameter space is shown. The 3σ upper bound on α_{21} from neutrino data is indicated by a red line. This limit has also been included as a prior in the results shown in the right panel. Here $\delta_{CP}^{\rm True}$ is fixed to $-\pi/2$ and the additional undisplayed parameters have been marginalized over. The allowed regions, darkest to lightest, correspond to 1σ to 4σ for 2 d.o.f., respectively.

Finally, we present an estimate of the absolute sensitivity of DUNE to the non-unitary parameter α_{21}. In order to do this, we extended our previous analysis, considering all the possible values of $\delta_{\rm CP}^{\rm True}$ and marginalizing over $\delta_{\rm CP}$ and ϕ_{21}. Fig. 6 shows the χ^2 profile obtained as a function of $|\alpha_{21}|$ after marginalizing over all the remaining parameters, including $\delta_{\rm CP}^{\rm True}$. The best fit point, denoted by a black point in the figure, is obtained for $|\alpha_{21}| = 3 \times 10^{-4}$. Nevertheless, the preference over the unitary hypothesis is not significant at all, as can be seen from the figure. The shaded band in Fig. 6 indicates the three benchmark values of α_{21} used in the analysis of CP sensitivity in DUNE (see the left panel of Fig. 4), while the horizontal dotted black line defines the parameter region allowed by DUNE at 90% of C.L., corresponding to the limit $|\alpha_{21}| < 0.046$. This bound is somewhat weaker than the constraints derived from neutrino oscillation searches, indicating that the analysis of long-baseline neutrino oscillations in DUNE is not expected to improve our current knowledge on the non-unitarity of the neutrino mixing matrix. However, it is worth mentioning that this constraint can also be regarded as independent and complementary to the bounds in Table I.

V. CONCLUSION AND DISCUSSION

We have reviewed the existing limits on non-unitarity parameters, from weak universality considerations as well as from neutrino oscillation data. We have discussed the model-

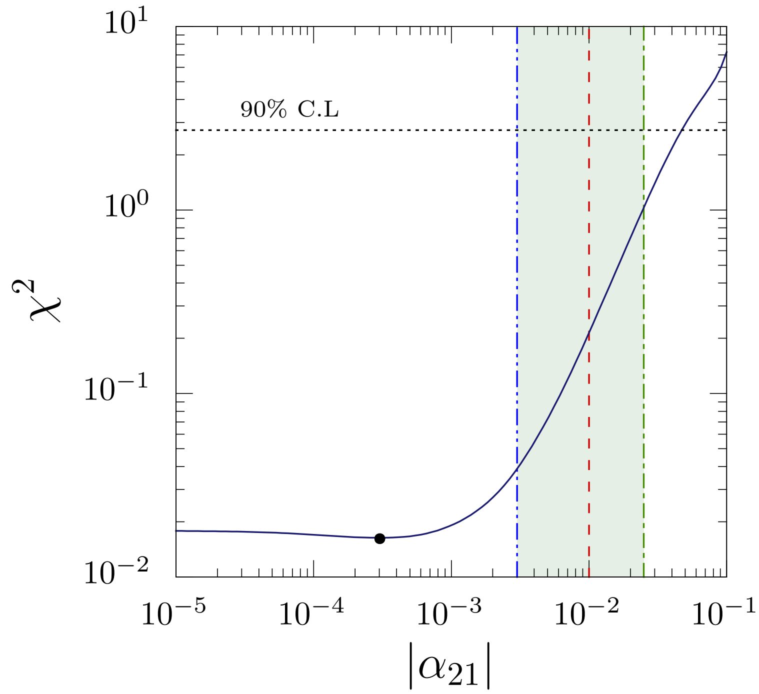

FIG. 6: DUNE sensitivity to α_{21} for arbitrary values of the Dirac CP phase. The expected sensitivity at 90% of C.L. is indicated by the horizontal line, while the three vertical lines correspond to the benchmark points considered in Fig. 4.

independent character of the latter constraints, since they only rely upon direct information from the neutrino sector, in contrast with the ones derived form charged lepton processes. We have developed in detail the formalism for neutrino propagation in matter in the presence of non-unitary neutrino mixing. In contrast to the standard unitary case, the neutral current potential contributes to the neutrino Hamiltonian in matter. Here we have focused our analysis on the case of the long-baseline neutrino experiment DUNE. First we have analyzed how the sensitivity to CP violation in DUNE can be affected by the presence of non-unitarity. We have found that DUNE's potential to probe CP violation is somewhat weakened, although not as much as one might have expected, see Fig. 4. The reason for this, apart from the high statistics, is mainly the fact that the DUNE experiment is characterized by a relatively wide beam, compared with current experiments. This nice feature partly mitigates the ambiguities stressed in [31]. Moreover, we have investigated how DUNE can probe neutrino properties beyond standard oscillations, such as the parameters characterizing non-unitarity, see Fig. 6. In this respect DUNE is not expected to perform better than previous short baseline oscillation searches at NOMAD, CHORUS and NuTeV. This discouraging result is not surprising, as the sensitivity to non-unitarity comes mainly from probing the "zero-distance effect" and hence involves "near" detection. This could be improved within a setup of the type suggested in Ref. [85].

Before closing, we mention two other recent related analyses. In Ref. [84] the authors considered the effect of extra neutrino states in neutrino oscillations, focusing on the differences and similarities between the case in which these neutrinos are kinematically accessible (sterile neutrinos) or not (non-unitary mixing matrix)[6]. They choose the stronger model-dependent bounds, for which the effect of non-unitarity on the neutrino signal in DUNE is very small and hence the loss in CP sensitivity. Finally, Ref. [92] suggested a novel possibility of discriminating sterile neutrinos and unitarity violation through CP violation.

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