Octant of $\theta_{23}$ in danger with a light sterile neutrino

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Present global fits of world neutrino data hint towards non-maximal $\theta_{23}$ with two nearly degenerate solutions, one in the lower octant ($\theta_{23} < \pi/4$), and the other in the higher octant ($\theta_{23} > \pi/4$). This octant ambiguity of $\theta_{23}$ is one of the fundamental issues in the neutrino sector, and its resolution is a crucial goal of next-generation long-baseline (LBL) experiments. In this letter, we address for the first time, the impact of a light eV-scale sterile neutrino towards such a measurement, taking the Deep Underground Neutrino Experiment (DUNE) as a case study. In the so-called 3+1 scheme involving three active and one sterile neutrinos, the $\nu_\mu \to \nu_e$ transition probability probes in the LBL experiments acquires a new interference term via active-sterile oscillations. We find that this interference term can mimic a swap of the $\theta_{23}$ octant, even if one uses the information from both neutrino and antineutrino channels. As a consequence, the sensitivity to the octant of $\theta_{23}$ can be completely lost, and this may have serious implications for our understanding of neutrinos from both the experimental and theoretical perspectives.

PACS numbers: 14.60.Pq, 14.60.St

Introduction. After the discovery of the smallest leptonic mixing angle $\theta_{13}$, the 3-flavor paradigm has been firmly established, and neutrino physics is entering the precision era. In the standard 3-flavor framework, the oscillations are governed by two mass-squared splittings $\Delta m^2_{21} \equiv m_2^2 - m_1^2$, and $\Delta m^2_{32} \equiv m_3^2 - m_2^2$, and three mixing angles ($\theta_{12}, \theta_{23}, \theta_{13}$). Two fundamental elements are still missing in this picture: the mass hierarchy (MH) and the CP-phase $\delta$, which, if $\neq (0, \pi)$, gives rise to leptonic CP-violation (CPV). A rich experimental program is underway to identify these two unknown properties, and to refine the estimates of the known mass-mixing parameters [1–5].

Current global neutrino data hint towards non-maximal $\theta_{23}$ with two nearly degenerate solutions: one $< \pi/4$, termed as lower octant (LO), and the other $> \pi/4$, denoted as higher octant (HO). The identification of the $\theta_{23}$ octant is a crucial goal in neutrino physics due to its deep implications for the theory of neutrino masses and mixing (see [6–10] for reviews). Notable models where the $\theta_{23}$ octant plays a key role are $\mu \leftrightarrow \tau$ symmetry [11–20], $A_4$ flavor symmetry [21–25], quark-lepton complementarity [26–29], and neutrino mixing anarchy [30–31]. From a phenomenological perspective, the information on the $\theta_{23}$ octant is also a vital input. In fact, it is well known that the identification of the two unknown properties (MH and CPV) is strictly intertwined with the determination of $\theta_{23}$ because of parameter degeneracy issues [32–34].

One of the most promising options to identify the $\theta_{23}$ octant is offered by the long-baseline (LBL) accelerator experiments. In these setups, a synergy between the $\nu_\mu \to \nu_e$ appearance and $\nu_\mu \to \nu_\mu$ disappearance channels exists [32–35], which confers an enhanced sensitivity to the $\theta_{23}$ octant. The $\nu_\mu \to \nu_e$ survival probability, at the leading order, depends on $\sin^2 2\theta_{23}$. Then, it is sensitive to deviations from maximality but is insensitive to the octant. On the other hand, the leading contribution to the $\nu_\mu \to \nu_\mu$ probability is proportional to $\sin^2 \theta_{23}$, and is thus sensitive to the octant. The combination of these two channels provides a synergistic information on $\theta_{23}$. A residual degeneracy persists between the $\theta_{23}$ octant and the CP-phase $\delta$, but it can be lifted with a balanced exposure of neutrino and antineutrino runs [36–37].

Most of the octant sensitivity studies have been performed within the 3-flavor framework (for recent works see [2, 37] [41–44]). However, there are strong indications that the standard picture may be incomplete. In particular, there is a number of short-baseline (SBL) anomalies which point towards the existence of new light eV-scale sterile neutrinos [45–47]. If this hypothesis gets confirmed, it may have important consequences for the 3-flavor searches. In fact, it has been already shown that the analysis of current LBL data is substantially affected by sterile neutrinos [48–49] and that the discovery reach of CPV and MH of prospective LBL data can be substantially deteriorated [50–51] albeit, at least for the future experiment DUNE, a residual sensitivity at an acceptable ($\sim 3\sigma$) level is preserved [51]. Recent studies of sterile

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1 Here, MH refers to the sign of $\Delta m^2_{31}$, which can be positive termed as normal hierarchy (NH), or negative denoted as inverted hierarchy (IH).
2 As shown in [11, 12], in the 3+1 scheme, the condition $\theta_{23} \approx 45^\circ$ implies an approximate realization of $\mu \leftrightarrow \tau$ symmetry, similarly to what happens in the standard 3-flavor scheme. Therefore, establishing that $\theta_{23}$ is maximal (non-maximal) would imply that $\mu \leftrightarrow \tau$ symmetry is unbroken (broken), irrespective of the existence of a light sterile neutrino.
neutrinos at LBL experiments can be found in [52–55].

In this letter we point out that the situation is much worse for the $\theta_{23}$ octant, whose determination is put in serious danger by the presence of active-sterile neutrino oscillations. Taking DUNE as a case study, we show that in the 3+1 scheme, the newly identified interference term \[ \text{that appears in the } \nu_\mu \to \nu_e \text{ transition probability} \] can mimic a swap of the $\theta_{23}$ octant. As a consequence, for unfavorable combinations of the CP-phases in the 4-flavor scheme, the sensitivity to the octant of $\theta_{23}$ can be completely lost.

**Theoretical framework.** In the 3+1 scheme, a fourth mass eigenstate $\nu_4$ is introduced and the mixing is described by a $4 \times 4$ matrix

\[ U = R_{34} R_{24} R_{14} R_{23} R_{13} R_{12}, \]

where $R_{ij}$ ($R_{ji}$) is a real (complex) rotation in the $(i,j)$ plane, which contains the $2 \times 2$ matrix

\[ R^2_{ij} = \begin{pmatrix} c_{ij} & s_{ij} \\ -s_{ij} & c_{ij} \end{pmatrix}, \quad R^2_{ji} = \begin{pmatrix} -s_{ij} c_{ij} & s_{ij} c_{ij} \\ -c_{ij} s_{ij} & c_{ij} s_{ij} \end{pmatrix}, \]

in the $(i,j)$ sub-block. For brevity, we have introduced the definitions

\[ c_{ij} \equiv \cos \theta_{ij}, \quad s_{ij} \equiv \sin \theta_{ij}, \quad \tilde{s}_{ij} \equiv s_{ij} e^{-i\delta_{ij}}. \]

Let us now come to the transition probability relevant for the LBL experiment DUNE. Matter effects have a sizable impact in DUNE, and confer a high sensitivity to the MH. However, for simplicity, we neglect them in the considerations below, because they are basically irrelevant for the physical process that we want to highlight. We stress that in the numerical simulations we properly include the matter effects assuming a line-averaged constant density of $2.87 \text{g/cm}^3$ based on the PREM profile of Earth crust. In [48], it has been shown that the 4-flavor probability can be approximated by the sum of three terms

\[ P_{\mu e}^{4\nu} \simeq P_0 + P_1 + P_2, \]

which in vacuum take the form

\[ P_0 \simeq 4s_{23}^2 s_{13}^2 \sin^2 \Delta, \]

\[ P_1 \simeq 8s_{13} s_{12} c_{12} s_{23} c_{23} (\alpha \Delta) \sin \Delta \cos (\Delta \pm \delta_{13}), \]

\[ P_2 \simeq 8s_{14} s_{24} s_{13} s_{23} \sin \Delta \sin (\Delta \pm \delta_{13} \mp \delta_{14}), \]

where $\Delta \equiv \Delta m_{31}^2 L/4E$ is the atmospheric oscillating frequency depending on the baseline $L$ and the neutrino energy $E$, and $\alpha \equiv \Delta m_{31}^2 / \Delta m_{21}^2$. The double sign in front of the CP-phases reflects the fact that it is opposite for neutrinos (upper sign) and antineutrinos (lower sign). The first term $P_0$, which is positive definite and independent of the CP-phases, gives the leading contribution to the probability. The term $P_1$ is related to the interference of the oscillations driven by the solar and atmospheric frequencies. This term, apart from higher order corrections, coincides with the standard interference term, which renders the 3-flavor transition probability sensitive to the CP-phase $\delta \equiv \delta_{13}$. The term $P_2$ is a genuine 4-flavor effect, and is driven by the interference between the atmospheric frequency and the large frequency related to the new mass eigenstate [48]. This term does not manifest an explicit dependency on $\Delta m_{41}^2 \equiv m_{41}^2 - m_{11}^2$ because the related oscillations are very fast and get averaged out by the finite energy resolution of the detector.

We now observe that, as can be inferred from the latest 3-flavor global analyses [50–55] and from the global 3+1 fits [56–58], the three small mixing angles have similar size $s_{13} \sim s_{14} \sim s_{24} \simeq 0.15$, and therefore they can all be assumed of the same order $\epsilon$, while the ratio $\alpha \simeq \pm 0.03$ is of order $\epsilon^2$. This implies that

\[ P_0 \sim \epsilon^2, \quad P_1 \sim \epsilon^3, \quad P_2 \sim \epsilon^3. \]

Now let us come to the $\theta_{23}$ octant issue. In general, we can re-express the atmospheric mixing angle as

\[ \theta_{23} = \frac{\pi}{4} \pm \eta, \]

where $\eta$ is a positive-definite angle and the positive (negative) sign corresponds to HO (LO). The current 3-flavor global fits [56–58] suggest that $\theta_{23}$ can deviate by no more than $\sim 6^\circ$ from maximal mixing. Equivalently, $\sin^2 \theta_{23}$ must lie in the range $\sim [0.4, 0.6]$. This implies that $\eta$ is confined to relatively small values ($\eta \lesssim 0.1$), and can be considered of the same order of magnitude ($\epsilon$) of $s_{13}$, $s_{14}$ and $s_{24}$. Therefore, it is legitimate to use the expansion

\[ s_{23}^2 = \frac{1}{2} (1 \pm \sin 2\eta) \simeq \frac{1}{2} \pm \eta. \]

An experiment can be sensitive to the octant if, despite the freedom introduced by the unknown CP-phases, there is still a difference between the probabilities in the two octants, i.e.

\[ \Delta P \equiv P^\text{HO}_{\mu e}(\delta_{13}^\text{HO}, \delta_{14}^\text{HO}) - P^\text{LO}_{\mu e}(\delta_{13}^\text{LO}, \delta_{14}^\text{LO}) \neq 0. \]

In Eq. (11) we must think to one of the two octants as the true choice, then for a given combination ($\delta_{13}^\text{HO}, \delta_{14}^\text{HO}$) there can be sensitivity to the octant if $\Delta P \neq 0$ in the hypothesis that ($\delta_{13}^\text{LO}, \delta_{14}^\text{LO}$) are both unknown and free to vary in the range $[-\pi, \pi]$. According to Eq. (4), we can split $\Delta P$ in the sum of three terms

\[ \Delta P = \Delta P_0 + \Delta P_1 + \Delta P_2. \]

The first term is positive-definite, does not depend on the CP-phases and is given by

\[ \Delta P_0 \simeq 8\eta s_{13}^2 \sin^2 \Delta. \]
The second and third terms depend on the CP-phases and can have both positive or negative values. Their expressions are given by

$$\Delta P_1 = A \left[ \cos(\Delta \pm \phi^{\text{HO}}) - \cos(\Delta \pm \phi^{\text{LO}}) \right], \quad (14)$$

$$\Delta P_2 = B \left[ \sin(\Delta \pm \psi^{\text{HO}}) - \sin(\Delta \pm \psi^{\text{LO}}) \right], \quad (15)$$

where for compactness, we have introduced the amplitudes$^3$

$$A = 4 s_{13} s_{12} c_{12} (\alpha \Delta) \sin \Delta, \quad (16)$$

$$B = 2 \sqrt{2} s_{14} s_{24} s_{13} \sin \Delta, \quad (17)$$

and the auxiliary CP-phases

$$\phi = \delta_{13}, \quad (18)$$

$$\psi = \delta_{13} - \delta_{14}, \quad (19)$$

with the appropriate superscripts (LO or HO). If we adopt as a benchmark value $\sin^2 \theta_{23} = 0.42$ (0.58) for LO (HO), i.e. $\eta = 0.08$, at the first oscillation maximum ($\Delta = \pi/2$), we have

$$\Delta P_0 \simeq 0.014, \quad |A| \simeq 0.013, \quad |B| \simeq 0.010. \quad (20)$$

These numbers give a feeling of the (similar) size of the three terms involved in Eq. (12). It is clear that an experiment can be sensitive to the octant only if the positive-definite difference $\Delta P_0$ cannot be completely compensated by a negative contribution coming from the sum of $\Delta P_1$ and $\Delta P_2$.

Now, we recall what happens in the 3-flavor framework, when the last term $\Delta P_2$ in Eq. (12) is absent. In this case, if one considers only the neutrino channel there are unfavorable combinations of the two CP-phases $\phi^{\text{LO}}$ and $\phi^{\text{HO}}$ for which $\Delta P = 0$ and there is no sensitivity to the octant. On the other hand, as recently recognized in\textsuperscript{37, 38}, the octant-$\delta_{13}$ degeneracy can be lifted if one exploits also the antineutrino channel. This fact can be understood from Fig. 1 which represents the bi-event plot for the DUNE experiment. In such a plot, the ellipses refer to the 3-flavor case, while the colored blobs represent the 3+1 scheme. We take $\sin^2 \theta_{23} = 0.42$ (0.58) as a benchmark value for the LO (HO). In the 3-flavor ellipses, the running parameter is $\delta_{13}$ varying in the range $[-\pi, \pi]$. In the 4-flavor blobs there are two running parameters, $\delta_{13}$ and $\delta_{14}$, both varying in their allowed ranges $[-\pi, \pi]$. In the 3+1 case we have assumed $\theta_{34} = 0^\circ$.

So we can fix the attention on one of the two hierarchies, for example the NH. We observe, that the (black) ellipse corresponding to the LO is well separated from the (yellow) HO ellipse. This separation is a synergistic effect of the fact that we are considering both neutrino and antineutrino events.

Finally, let us come to the 3+1 scheme. In this case the third term in Eq. (12) is active. It depends on the additional CP-phase $\delta_{14}$, so its sign can be chosen independently of that of the second term. This circumstance gives more freedom in the 3+1 scheme and there is more space for degeneracy. The bi-event plot in Fig. 1 confirms such a basic expectation. The graph now becomes a blob, which can be seen as a convolution of an ensemble of ellipses (see\textsuperscript{50}), and the separation between LO and HO is lost even if one considers both neutrino and antineutrino events.

**Numerical results.** In our simulations, we use the GLoBES software\textsuperscript{51, 62}. For DUNE, we consider a total exposure of 248 kt · MW · year, shared equally between neutrino and antineutrino modes. For the details of the DUNE setup, and of the statistical analysis, we refer the reader to our recent paper\textsuperscript{51}, and references therein. Figure 2 displays the discovery potential for identifying the true octant as a function of true $\delta_{13}$. The left (right) panel refers to the true choice LO-NH (HO-NH). In both panels, for comparison, we show the results for the 3-flavor case (represented by the black curve). Concerning the 3+1 scheme, we draw the curves.

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$^3$ In the expressions of $A$ and $B$ we are neglecting terms proportional to powers of $\eta$, which would give rise to negligible (at least fourth order in $\epsilon$) corrections.

$^4$ The small overlap between NH and IH blobs in Fig. 1 for the LO case can be removed using the spectral information available in DUNE (see\textsuperscript{51}).
corresponding to four representative values of true $\delta_{14}$ ($0^\circ, 180^\circ, -90^\circ, 90^\circ$). In the 3$\nu$ case we marginalize over ($\theta_{23}, \delta_{13}$) (test). In the 3+1 scheme, we fix $\theta_{14} = 0$, and marginalize over ($\theta_{23}, \delta_{13}, \delta_{14}$) (test).

The 3-flavor curves have been already discussed in the literature (see for example 2, 37, 44). Nonetheless, we deem it useful to make the following remarks: i) a good $\theta_{23}$ octant sensitivity for all values of $\delta_{13}$ (true) can be achieved with equal neutrino and antineutrino runs [37], ii) the spectral information plays an important role in distinguishing between the two octants for unfavorable choices of true hierarchy and $\delta_{13}$, and iii) always the sensitivity is higher for LO compared to HO irrespective of the hierarchy choice. For the first time, during this work, we realized that this last issue of asymmetric sensitivity between LO and HO is related to a synergistic effect of the $\nu_\mu \rightarrow \nu_\mu$ and $\nu_\mu \rightarrow \nu_e$ channels. Basically, the $\nu_\mu \rightarrow \nu_\mu$ channel fixes the test value of $\theta_{23}$ in the octant opposite to its true value. However, such a test value is not exactly equal to its octant symmetric choice (i.e., $\theta_{23}^{\text{test}} \neq \pi/2 - \theta_{23}^{\text{true}}$). This happens because the $\nu_\mu \rightarrow \nu_\mu$ survival probability contains higher order octant-sensitive terms, which can be probed in high-statistics experiments like DUNE. We find that these corrections always go in the direction of increasing (decreasing) the difference $|\sin^2 \theta_{23}^{\text{test}} - \sin^2 \theta_{23}^{\text{true}}|$ by $\sim 15\%$ with respect to its default value $|0.58 - 0.42| = 0.16$ in the LO (HO) case. Since the leading term of the $\nu_\mu \rightarrow \nu_e$ appearance channel is sensitive to this difference, the performance is enhanced (suppressed) in the LO (HO) case.

Fig. 2 shows that in the 3+1 scheme there exist unfavorable combinations of $\delta_{13}$ (true) and $\delta_{14}$ (true) for which the octant sensitivity falls below the 2$\sigma$ level. We have verified that for such combinations the spectra corresponding to the two octants are almost indistinguishable both for neutrinos and antineutrinos. Therefore, even a broad-band experiment such as DUNE cannot break the degeneracy introduced by a sterile neutrino.

So far, we have considered two true values of $\sin^2 \theta_{23} = 0.42$ (LO) and 0.58 (HO) (see Fig. 2). However, it is interesting to ask how things change if different choices are made for the true value of $\theta_{23}$. Figure 3 answers this question. It represents the discovery potential for identifying the true octant in the plane $[\sin^2 \theta_{23}, \delta_{13}]$ (true) assuming NH as true choice. The left (right) panel corresponds to the 3$\nu$ (3+1) scheme. In the 3+1 case we marginalize away also the CP-phase $\delta_{14}$ (true) (in addition to all the test parameters) since it is unknown. Hence, the outcome of this procedure determines the minimal guaranteed sensitivity, i.e. the one corresponding to the worst case scenario. The solid blue, dashed magenta, and dotted black curves correspond, respectively, to $2\sigma$, $3\sigma$, and $4\sigma$ confidence levels (1 d.o.f.). The comparison of the two panels gives a bird-eye view of the situation. It is clear that, in the 3+1 scheme, no minimal sensitivity is guaranteed in the entire plane. We have checked that similar conclusions are valid also in the case of IH as true MH.

**Conclusions.** In this letter, we have addressed for the first time the impact of a light eV-scale sterile neutrino in identifying the octant of the mixing angle $\theta_{23}$ at the next generation LBL experiment DUNE. We have shown that in the 3+1 scheme, the new recently identified interference term 48 that enters the $\nu_\mu \rightarrow \nu_e$ transition probability can perfectly mimic a swap of the $\theta_{23}$ octant, even when we use the information from both the neu-
trino and antineutrino channels. As a consequence, the sensitivity to the octant of $\theta_{23}$ can be completely lost in the presence of active-sterile oscillations. It remains to be seen if other kinds of experiments, in particular those using atmospheric neutrinos, can lift or at least alleviate the degeneracy that we have found in the context of LBL experiments. Our educated guess is that this would prove to be very difficult since obtaining a satisfying $\theta_{23}$ octant sensitivity with atmospheric neutrinos is a very hard task already in the 3-flavor framework, and in the enlarged 3+1 scheme, the situation should naturally worsen. At the end, we just want to emphasize the fact that the presence of light sterile neutrinos will have far-reaching consequences on the physical effects that we are going to observe in future long-baseline experiments such as DUNE, and we may land up with a different interpretation of the measured event spectra.

Acknowledgments

S.K.A. is supported by the DST/INSPIRE Research Grant [IFA-PH-12], Department of Science & Technology, India. A part of S.K.A.’s work was carried out at the International Centre for Theoretical Physics (ICTP), Trieste, Italy. It is a pleasure for him to thank the ICTP for the hospitality and support during his visit via SIMIONS Associateship. A.P. is supported by the grant “Future In Research” Beyond three neutrino families, Fondo di Sviluppo e Coesione 2007-2013, APQ Ricerca Regione Puglia, Italy, Programma regionale a sostegno della specializzazione intelligente e della sostenibilità sociale ed ambientale. A.P. acknowledges partial support by the research project TAsP funded by the Instituto Nazionale di Fisica Nucleare (INFN).

Note added

After the completion of this work, the IceCube [63], Daya Bay [64], and MINOS [65] Collaborations reported new constraints on active-sterile mixing. The new upper limit from the IceCube Collaboration [63] on $\sin^2 2\theta_{24}$ around the current best-fit $\Delta m^2_{41} \approx 1.75$ eV$^2$ [66] is $\approx 0.2$ at 99% confidence level, which means that $\theta_{24}$ is constrained to be smaller than 13$^\circ$ or so. The MINOS Collaboration placed a new upper limit of 0.03 on $\sin^2 2\theta_{24}$ around $\Delta m^2_{41} \approx 1.75$ eV$^2$ at 90% C.L. [66] suggesting that the upper limit on $\theta_{24}$ is around 10$^\circ$. Therefore, the benchmark value $\theta_{24} = 9^\circ$ which we have considered in our work is compatible with these new limits. The combined analysis of the Daya Bay and Bugey-3 data provides a new constraint [67] on $\sin^2 2\theta_{14}$ which is $\approx 0.06$ at 90% confidence level around $\Delta m^2_{41} \approx 1.75$ eV$^2$. This implies that $\theta_{14}$ is smaller than 7$^\circ$ or so, which is pretty close to the benchmark value of $\theta_{14} = 9^\circ$ that we have considered in our analysis. For completeness, we have explicitly checked performing new simulations that our results remain almost unaltered if we take $\theta_{14} = 7^\circ$ and $\theta_{24} = 9^\circ$ instead of our benchmark choice of $\theta_{14} = \theta_{24} = 9^\circ$. Hence, we can safely conclude that the sensitivity towards the octant of $\theta_{23}$ can be completely lost even in light of the new constraints on the active-sterile mixing that were reported recently.

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