Geometry of the neutrino mixing space

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We study the geometric structure of the physical region of neutrino mixing matrices as part of the unit ball of the spectral norm. Each matrix from the geometric region is a convex combination of unitary PMNS matrices. The disjoint subsets corresponding to a different minimal number of additional neutrinos are described as relative interiors of faces of the unit ball. We determined the Carathéodory's number showing that at most four unitary matrices of dimension three are necessary to represent any matrix from the neutrino geometric region. For matrices which correspond to scenarios with one and two additional neutrino states, the Carathéodory's number is two and three, respectively. Further, we discuss the volume associated with different mathematical structures, particularly with unitary and orthogonal groups, and the unit ball of the spectral norm. We compare the obtained volumes to the volume of the region of physically admissible mixing matrices for both the *CP*-conserving and *CP*-violating cases in the present scenario with three neutrino families and scenarios with the neutrino mixing matrix of dimension higher than three.

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I. INTRODUCTION

Over the years neutrino oscillation experiments have provided in-depth information about the structure of the neutrino standard 3×3 unitary mixing matrix U_{PMNS} [1,2]. We know already that the θ_{13} mixing angle is nonzero, and as a consequence, the (1,3) element of U_{PMNS} is also nonzero [3–5]. In that way, the tri-bimaximal mixing structure has been excluded [6]. Recently a lot of attention is given to the study of the value of the neutrino *CP* complex phase. If it is nonzero it could shed a new light on the matter-antimatter problem [7]. On top of that, there is a possibility that more than three known neutrinos exist. In this case new neutrino states, commonly known as sterile neutrinos, can mix with active Standard Model neutrinos. This implies that the 3×3 neutrino mixing matrix is no longer unitary. There are various approaches to deal with the non-unitarity problem, for instance a decomposition of a general matrix into a product with a unitary matrix are considered. The two often used approaches are known as the α and η parametrizations [8–13]. In the α parametrization's framework a small deviation from unitarity is encoded into a lower triangular matrix, whereas in the η framework, possible deviations from unitarity are encoded in a Hermitian matrix. In Ref. [14] a different approach was proposed based on matrix theory where the experimentally established interval neutrino mixing matrix U_{int} is studied using matrix theory methods, and its connections to the non-standard neutrino physics have been established by exploring singular values and contractions. In [15] the matrix theory has been applied to phenomenological studies and new limits on light-heavy neutrino mixings in the $3 + 1$ model (three light, known neutrinos with one additional sterile neutrino) have been obtained. In another work where the matrix theory methods have been explored in the context of neutrino physics, conditions for the existence of the gap in the seesaw mass spectrum have been established and justified [16,17]. We should also mention that an interesting mathematical connection between eigenvalues and eigenvectors has been rediscovered in the context of neutrino oscillations in matter [18,19]. There has been also attempts to predict neutrino masses by geometric and topological methods. In [20] the neutrino mass spectrum is explored through the model of cosmological evolution based on exotic smooth structures. In this work we focus on further geometrically based studies toward the understanding of the class of physically admissible neutrino mixing matrices where the 3×3 mixing matrix could be a part of a higher dimensional unitary mixing matrix. Our aim is to study the structure of a geometric region Ω that corresponds to physically admissible mixing matrices, which has been introduced in [14].

In the next chapter we give a general setting for our discussion introducing a neutrino mixing matrix and current experimental limits for the mixing parameters. In the third chapter, we define the region of physically

admissible mixing matrices and its subsets corresponding to a different minimal number of additional neutrinos. In the fourth chapter, we recognize the geometric region as a subset of the unit ball of a spectral norm and describe its facial structure. Next, we will connect the facial structure of Ω to the minimal number of additional sterile neutrinos and we will determine the so-called Carathéodory number which informs us about a minimal number of unitary 3×3 matrices which are needed to span the whole Ω space for a given number of sterile neutrinos. This allows for an optimal construction of physical mixing matrices that can be used for further analysis of scenarios involving sterile neutrinos. Finally, we determine the volume of this region for CP conserving and violating cases. The article is finished with a summary and outlook. The main text is supported by the Appendix containing auxiliary definitions and theorems.

II. SETTING: NEUTRINO MIXING MATRIX AND EXPERIMENTAL DATA

Neutrino flavor fields are (linear) combinations of the massive fields

$$\nu_l^f = \sum_{i=1}^{n} U_{li} \nu_i^m. \tag{1}$$

This property of neutrino fields is called the neutrino mixing mechanism. The mixing of neutrinos occurs regardless if they are Dirac or Majorana particles [21,22]. As the massive and flavor fields form two orthogonal bases in the state space, the transition from one base to another can be done by a unitary matrix. This restricts coefficients of the linear combination, the sum of squares of their absolute values must equal one

$$\nu_l^f = \sum_{i=1}^{n} U_{li} \nu_i^m \quad \text{with} \quad \sum_{i=1}^{n} |U_{li}|^2 = 1. \tag{2}$$

For $n = 3$ in (1), the 3×3 unitary matrix U corresponding to three light known neutrino mixing is known as the PMNS mixing matrix [23,24]. The general $n \times n$ complex matrix has n^2 complex parameters or equivalently $2n^2$ real parameters. The unitarity condition $UU^\dagger = I$ imposes additional n^2 constraints on the elements. It can be seen from $UU^\dagger$ which is a Hermitian matrix and has n independent diagonal elements and $n^2 - n$ independent off-diagonal elements which together give n^2 independent elements or conditions imposed on the unitary matrix. Thus, the $n \times n$ unitary matrix has $2n^2 - n^2 = n^2$ independent real parameters. An alternative way to see this is by writing a unitary matrix as the matrix exponent of the Hermitian matrix, i.e., $U = e^{iH}$, where the H matrix is Hermitian and thus has n^2 independent real parameters which implies that U also has n^2 independent real parameters. These parameters can be split into two categories: rotation angles and complex phases. The number of angles corresponds to the number of parameters of the orthogonal matrix which has $\frac{n(n-1)}{2}$ independent real parameters. The remaining parameters correspond to phases. Thus, the n^2 independent real parameters of the unitary matrix split into

$$\begin{aligned} \text{angles}&: \frac{n(n-1)}{2}, \\ \text{phases}&: \frac{n(n+1)}{2}. \end{aligned} \tag{3}$$

However, not all phases are physical observables. The charged leptons and neutrino fields can be redefined as

$$\nu_i \to e^{i\alpha_i} \nu_i \quad \text{and} \quad l \to e^{i\beta_l} l. \tag{4}$$

The α_i and β_l phases can be chosen in such a way that they eliminate $2n - 1$ phases from the mixing matrix leaving the Lagrangian invariant. This reduces the number of phases of the mixing matrix. The number of remaining free parameters is $(n-1)^2$ which divides into

$$\begin{aligned} \text{angles}&: \frac{n(n-1)}{2}, \\ \text{phases}&: \frac{(n-1)(n-2)}{2}. \end{aligned} \tag{5}$$

These are the numbers under consideration when neutrinos are of the Dirac type. However, neutrinos can also be particles of the Majorana type. Then the Majorana condition $\nu_i^{\mathcal{C}} = \nu_i$ where $\mathcal{C}$ is the charge conjugate operator, fixes phases of the neutrino fields, which no longer can be chosen to eliminate phases in the mixing matrix. On the other hand, the phases of charged leptons are still arbitrary and can be chosen in such a way as to eliminate phases from the mixing matrix. Thus, from all $\frac{n(n+1)}{2}$ phases of the unitary matrix, n phases can be eliminated. Finally, for the Majorana neutrinos, the number of free parameters of the mixing matrix is as follows

$$\begin{aligned} \text{angles}&: \frac{n(n-1)}{2}, \\ \text{phases}&: \frac{n(n-1)}{2}. \end{aligned} \tag{6}$$

Knowing the number of parameters necessary to describe the mixing matrix, we can find its explicit form by invoking a particular parametrization. In the minimal scenario, the mixing matrix is a 3×3 matrix and thus for the Dirac case we have three mixing angles and one complex phase. The standard way of parametrizing the PMNS mixing matrix is as the product of three rotation

matrices with additional complex phase in one of them, i.e., in terms of Euler angles θ_{12}, θ_{13}, θ_{23} and complex phase δ

$$U_{\mathrm{PMNS}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta} \\ 0 & 1 & 0 \\ -s_{13}e^{i\delta} & 0 & c_{13} \end{pmatrix} \times \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \equiv \begin{pmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3} \\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3} \end{pmatrix}. \tag{7}$$

In the case of Majorana neutrinos we must include additional phases, which is done typically by multiplying the PMNS mixing matrix from the right-hand side by a diagonal matrix of phases P^M. For the 3×3 mixing matrix, we must add two more complex phases. The Majorana neutrino mixing matrix is then given by

$$U^M_{\mathrm{PMNS}} = U_{\mathrm{PMNS}} P^M, \quad \text{where } P^M = \mathrm{diag}(e^{i\gamma_1}, e^{i\gamma_2}, 1). \tag{8}$$

Oscillation experiments provide the major information about the structure of the neutrino mixing matrix. The current data gives the following limits for the mixing parameters [1,2]

$$\theta_{12} \in [31.27°, 35.86°], \qquad \theta_{23} \in [40.1°, 51.7°],$$
$$\theta_{13} \in [8.20°, 8.93°], \qquad \delta \in [120°, 369°]. \tag{9}$$

The global fits to oscillation experiments give the following allowed ranges for *the absolute values* of mixing matrix elements [2] (at the 3σ confidence level)

$$|U|_{3\sigma} = \begin{pmatrix} [0.801, 0.845] & [0.513, 0.579] & [0.143, 0.155] \\ [0.243, 0.500] & [0.471, 0.689] & [0.637, 0.776] \\ [0.271, 0.525] & [0.477, 0.694] & [0.613, 0.756] \end{pmatrix}. \tag{10}$$

To get exact values of the allowed ranges we imputed the allowed ranges of parameters (9) into the parametrization (7), which in the *CP* invariant case give the following interval matrix

$$O_{\mathrm{int}} = \begin{pmatrix} [0.801, 0.845] & [0.513, 0.579] & [0.143, 0.155] \\ [-0.529, -0.417] & [0.431, 0.606] & [0.637, 0.776] \\ [0.233, 0.388] & [-0.721, -0.586] & [0.613, 0.756] \end{pmatrix}, \tag{11}$$

whereas when the nonzero *CP* phase δ is included, the elements of the U_{int} are within the following ranges

$$\begin{aligned} U_{e1} &\in [0.801, 0.845], \\ U_{e2} &\in [0.513, 0.579], \\ U_{e3} &\in [-0.155 - 0.155i, 0.155 + 0.134i], \\ U_{\mu 1} &\in [-0.528 - 0.0901i, -0.218 + 0.104i], \\ U_{\mu 2} &\in [0.432 - 0.0616i, 0.707 + 0.0711i], \\ U_{\mu 3} &\in [0.637, 0.776], \\ U_{\tau 1} &\in [0.233 - 0.0878i, 0.538 + 0.101i], \\ U_{\tau 2} &\in [-0.721 - 0.060i, -0.453 + 0.0693i], \\ U_{\tau 3} &\in [0.613, 0.756]. \end{aligned} \tag{12}$$

Though the experimental results given in (11) and (12) are based on the U_{PMNS} matrix (7), we can reverse the problem and ask the following question: What can we learn about a geometrical structure of a region of physical mixing matrices, not restricted to U_{PMNS}, given basic mixings between light known neutrinos in (11) or (12)?

We will answer this question in the following sections.

III. REGION OF PHYSICALLY ADMISSIBLE MIXING MATRICES

We are interested in a special class of matrices encompassing unitary matrices or matrices which can be a submatrix of a unitary matrix. These are known as contractions and are defined by the following formula $\|A\| \leq 1$ (for necessary definitions see Appendix A). The importance of contractions in neutrino mixing studies and their properties have been discussed in [14,15].

We will show that a matrix constructed as a finite convex combination of unitary matrices is a contraction. Let U_i, $i = 1, \ldots, n$, be a unitary matrix, and let $A = \sum_{i=1}^n \alpha_i U_i$ with

$\alpha_i \geq 0$ and $\sum_{i=1}^n \alpha_i = 1$, then

$$\|A\| = \|\sum_{i=1}^n \alpha_i U_i\| \leq \sum_{i=1}^n \alpha_i \|U_i\| = \sum_{i=1}^n \alpha_i = 1 \Rightarrow \|A\| \leq 1. \tag{13}$$

The converse is also true [25], thus we have

Theorem III.1: A matrix A is a contraction if and only if A is a finite convex combination of unitary matrices.

This characterization of contractions has physical consequences. It allows to gather physically meaningful mixing matrices into a geometric region.

Definition 1: The region of all physically admissible mixing matrices, denoted Ω, is the set of all finite convex combinations of 3×3 unitary matrices with parameters restricted by experiments

$$\Omega := \mathrm{conv}(U_{\mathrm{PMNS}}) = \left\{ \sum_{i=1}^{m} \alpha_i U_i | U_i \in U(3), \alpha_1, \ldots, \alpha_m \geq 0, \sum_{i=1}^{m} \alpha_i = 1, \theta_{12}, \theta_{13}, \theta_{23} \text{ and } \delta \text{ given by experimental values} \right\}. \tag{14}$$

There is another equivalent definition of the Ω region, which reflects its geometric nature, namely as the convex hull spanned on the unitary PMNS matrices.

The Corollary 1 given in Appendix B restricts the minimal dimension of the unitary extension of the contractions. This allows us to divide the Ω region into four disjoint subsets according to the minimal dimension of the unitary dilation

$$\Omega_1 : 3+1 \text{ scenario} : \Sigma = \{\sigma_1 = 1, \sigma_2 = 1, \sigma_3 < 1\}, \tag{15}$$

$$\Omega_2 : 3+2 \text{ scenario} : \Sigma = \{\sigma_1 = 1, \sigma_2 < 1, \sigma_3 < 1\}, \tag{16}$$

$$\Omega_3 : 3+3 \text{ scenario} : \Sigma = \{\sigma_1 < 1, \sigma_2 < 1, \sigma_3 < 1\}, \tag{17}$$

$$\Omega_4 : \text{PMNS scenario} : \Sigma = \{\sigma_1 = 1, \sigma_2 = 1, \sigma_3 = 1\}. \tag{18}$$

This division allows to analyze individually scenarios with a different number of sterile neutrinos. Thus, the study of geometric features of this region gives a possibility for a better understanding of neutrino physics, especially regarding the number of additional sterile neutrinos and the structure of the complete mixing matrix.

It is important to notice that matrices from the Ω_1 subset can be extended to unitary matrices of arbitrary dimension, starting from the dimension four. The same is true for contractions from the subset Ω_2 which can produce any unitary matrices of dimension five or higher. It may look that there is an overlapping between matrices from different subsets of the Ω region and some of them may be redundant. This is however not true, as unitary matrices produced by the contraction from each subset are not overlapping. It is so because contractions must end up in the 3×3 top diagonal block of a complete unitary matrix and as the subsets are disjoint, we cannot reproduce the same unitary matrices using contractions from different subsets. Thus, instead of overlapping, we should treat dilations of a given dimension of contractions from different subsets as complementary to each other.

IV. GEOMETRY OF THE REGION OF PHYSICALLY ADMISSIBLE MIXING MATRICES

The Ω region is a subset of the unit ball of the spectral norm

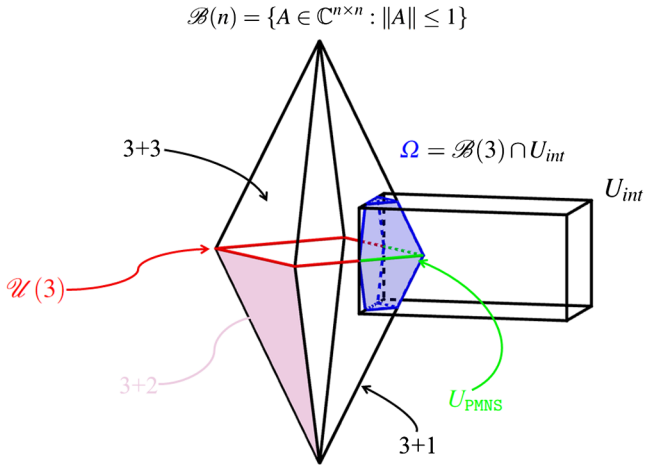

FIG. 1. Schematic visualization of the region of physically admissible mixing matrices as an intersection of $\mathcal{B}(3)$ and U_{int}. The double pyramid shape corresponds to the unit ball of a spectral norm. Its middle circumference, in red, represents its extreme points, i.e., $\mathcal{U}(3)$ group. Its edges and sides represent contractions with a minimal unitary extension, 4×4 and 5×5, respectively. Whereas the interior of $\mathcal{B}(3)$ corresponds to the contraction that minimally can be extended to 6×6 unitary matrices. The cuboid represents a hypercube of the interval matrix U_{int}. At the intersection of these two structures is the Ω region, in blue, and the set of PMNS mixing matrices is highlighted in green.

$$\mathcal{B}(n) = \{A \in \mathbb{C}^{n\times n} : \|A\| \leq 1\}. \tag{19}$$

This fact allows us to give another characterization of the Ω region as the intersection of the $\mathcal{B}(3)$ with the interval matrix U_{int} in Eqs. (11)–(12), i.e.,

$$\Omega = \mathcal{B}(3) \cap U_{\mathrm{int}}. \tag{20}$$

The relation between Ω and other involved geometric structures is visualized in Fig. 1.

The geometry of $\mathcal{B}(n)$ is strictly connected to the geometry of symmetric gauge functions [26].

Definition 2: A function $\Phi : \mathbb{R}^n \to \mathbb{R}$ is a symmetric gauge function if it satisfies the following conditions

(1) Φ is a vector norm,
(2) For any permutation matrix P we have $\Phi(Px) = \Phi(x)$,
(3) $\Phi(|x|) = \Phi(x)$.

Von Neumann proved that symmetric gauge functions and unitarily invariant norms (A2) are connected to each other [27], namely

Theorem IV.1: $\|\cdot\|$ is a unitary invariant norm if and only if there exists a symmetric gauge function Φ such that $\|A\| = \Phi(S(A))$ for all $A \in \mathbb{C}^{n\times n}$, where $S(A)$ is the set of singular values of A.

The spectral norm is a unitarily invariant norm and its corresponding symmetric gauge function is an infinite norm, i.e.,

$$\Phi_\infty(x) = \max\{|x_1|, |x_2|, \ldots, |x_n|\}. \quad (21)$$

The unit ball of the infinite norm is a hypercube

$$\mathcal{B}_\infty(n) = \{x \in \mathbb{R}^n : \Phi_\infty(x) \leq 1\} = [-1, 1]^n. \quad (22)$$

The connection between spectral norm and infinity norm is used in the proof of Proposition V.1.

The Von Neuman's relation between unitary invariant norms and symmetric gauge functions is also reflected in the geometry of the corresponding unit balls. The characterization of the extreme points and facial structure of unit balls of unitarily invariant norms by the corresponding structure of unit balls of symmetric gauge functions have been studied in [28–32]. Faces and extreme points are defined as follows [33,34]

Definition 3: Let $C \in \mathbb{R}^n$ be a convex set. A convex set $F \subseteq C$ is called a face of C if for every $x \in F$ and every $y, z \in C$ such that $x \in (y, z)$, we have $y, z \in F$.

Definition 4: The zero dimensional faces of a convex set C are called extreme points of C. Thus a point $x \in C$ is an extreme point of C if and only if there is no way to express x as a convex combination $(1-\lambda)y + \lambda z$ such that $y, z \in C$ and $0 < \lambda < 1$, except by taking $x = y = z$.

It appears that the extreme points of the $\mathcal{B}(n)$ are exactly unitary matrices. This result has also been obtained in a more general setting by Stoer [35]. The facial structure of the $\mathcal{B}(n)$ is given in the following theorem [29,32]

Theorem IV.2: $\mathcal{F}$ is a face of $\mathcal{B}(n)$ if and only if there exist $0 \leq r \leq n$ and unitary matrices U and V such that

$$\mathcal{F} = \left\{ U \begin{pmatrix} I_r & 0 \\ 0 & A \end{pmatrix} V : A \in \mathcal{B}(n-r) \right\}. \quad (23)$$

As the Ω region in Eq. (20) is a subset of $\mathcal{B}(3)$, its geometric structure is inherited from $\mathcal{B}(3)$. Thus, the facial structure of the Ω region is the same as for $\mathcal{B}(3)$ with restriction of parameters of unitary matrices U and V to experimental results in Eq. (9) and with established ranges of singular values

CP invariant scenario:

$$\{\sigma_1 = 0.95954, \sigma_2 = 0.88186, \sigma_3 = 0.84189\},$$

General scenario:

$$\{\sigma_1 = 0.95592, \sigma_2 = 0.84112, \sigma_3 = 0.70275\}. \quad (24)$$

The faces of $\mathcal{B}(3)$ defined in Eq. (23) do not correspond entirely to physically interesting subsets in Eqs. (15)–(17) of Ω. Namely, higher-dimensional faces contain lower-dimensional faces, e.g., for $r = 1$ the face contains not only matrices with two singular values strictly less than one, but also unitary matrices and contractions with only one singular value strictly less than one. In other words faces of $\mathcal{B}(3)$ comprise matrices from different subsets of Ω. To restrict faces to subsets containing only matrices with the specific number of singular values strictly less than one, we can use the notion of the relative interior [33].

Definition 5.: The relative interior of a convex set $C \subset \mathbb{R}^n$, which is denoted by $ri(C)$, is defined as the interior which results when C is regarded as a subset of its affine hull $\mathrm{aff}(C)$.

In this definition by the affine hull of the set C we understand the set of all finite affine combinations of elements of C [36], i.e., $\mathrm{aff}(C) = \{\sum_{i=1}^k \alpha_i x_i : x_i \in C, \sum_{i=1}^k \alpha_i = 1\}$. In that way, the subsets of $\mathcal{B}(n)$ corresponding to different minimal unitary extensions are the relative interiors of $\mathcal{F}$, i.e., subsets of faces for which singular values of the A submatrix are strictly smaller than one.

Definition 6: The subsets $\Omega_1, \ldots, \Omega_4$ of the Ω region are relative interiors of the faces $\mathcal{F}$ of $\mathcal{B}(3)$ for $r = 2, 1, 0, 3$, respectively, with parameters of unitary matrices U and V restricted by experimental data and with allowed ranges of singular values.

There is another way to characterize subsets of the Ω region, namely in terms of Ky-Fan k-norms.

Definition 7: For a given matrix $A \in \mathbb{C}^{n\times n}$ the Ky-Fan k-norm is defined as the sum of k largest singular values

$$\|A\|_k = \sum_{i=1}^k \sigma_i(A), \quad \text{for } k = 1, \ldots, n. \quad (25)$$

In particular for matrices in $\mathbb{C}^{3\times 3}$ the three possible Ky-Fan norms are

$$\begin{aligned} \|A\|_1 &= \sigma_1(A) \text{ (spectral norm)}, \\ \|A\|_2 &= \sigma_1(A) + \sigma_2(A), \\ \|A\|_3 &= \sigma_1(A) + \sigma_2(A) + \sigma_3(A) \text{ (nuclear norm)}. \end{aligned} \quad (26)$$

Let us define for $k = 1, \ldots, 3$ the following sets

$$\begin{aligned} S_k(r) &= \{A \in \mathbb{C}^{n\times n} : \|A\|_k = r\}, \\ A_k(r_1, r_2) &= \{A \in \mathbb{C}^{n\times n} : r_1 \leq \|A\|_k < r_2\}, \end{aligned} \quad (27)$$

i.e., we defined the sphere of radius r and the annulus with radii r_1 and r_2 for Ky-Fan norms centered at the origin. Then, the subsets of the Ω can be defined as

$$\begin{aligned} \Omega_1 &= S_1(1) \cap S_2(2) \cap A_3(2 + \sigma_{3\,\min}, 3), \\ \Omega_2 &= S_1(1) \cap A_2(1 + \sigma_{2\,\min}, 2) \cap A_3(1 + \sigma_{2\,\min} + \sigma_{3\,\min}, 3), \\ \Omega_3 &= A_1(\sigma_{1\,\min}, 1) \cap A_2(\sigma_{1\,\min} + \sigma_{2\,\min}, 2) \\ &\quad \cap A_3(\sigma_{1\,\min} + \sigma_{2\,\min} + \sigma_{3\,\min}, 3), \\ \Omega_4 &= S_1(1) \cap S_2(2) \cap S_3(3), \end{aligned} \quad (28)$$

where $\sigma_{i\,\min}$ for $i = 1, 2, 3$ are lower limits of singular values allowed by current experimental data (24).

We have described the subsets of the Ω region corresponding to a different number of additional neutrinos as relative interiors of the unit ball of the spectral norm with restricted range of parameters. In this way we established a correspondence between the geometry of Ω and $\mathcal{B}(3)$. This will allow us to study the further properties of the region of physically admissible mixing matrices by geometric tools used for unit balls of matrix norms and gauge symmetric functions.

V. PHYSICALLY ADMISSIBLE MIXING MATRICES AS CONVEX COMBINATIONS OF PMNS MATRICES

The Ω region (14) is defined as the convex hull of unitary PMNS mixing matrices or equivalently as the set of a finite convex combination of PMNS mixing matrices. In this way, we claim that every physically admissible mixing matrix can be represented as a finite convex combination of unitary PMNS matrices. This agrees with the Krein-Milman theorem which states [36,37]

Theorem V.1: Let $C \subset \mathbb{R}^n$ be a nonempty compact convex set, and let $\mathrm{ext}(C)$ be the set of extreme points of C, then

$$C = \overline{\mathrm{conv}}(\mathrm{ext}(C)), \tag{29}$$

where bar over conv means a closure. As we have discussed, the extreme points of the unit ball of the spectral norm are unitary matrices and as the Ω is a subset of the $\mathcal{B}(3)$, the above theorem justifies our definition. However, this theorem does not put any restriction on the number of extreme points necessary to construct any point of a convex set as a convex combination of its extreme points. The upper bound for this number has been given by Carathéodory [36,38].

Theorem V.2: If $K \subset \mathbb{R}^n$, then each point of $\mathrm{conv}(K)$ is a convex combination of at most $n+1$ points of K.

The natural question arises: What is the Carathéodory number for the $\mathcal{B}(n)$ and Ω which are embedded in $\mathbb{C}^{n^2} \simeq \mathbb{R}^{2n^2}$? In the physically interesting case where $n=3$ according to the Carathéodory theorem we would need 19 unitary matrices. However, we will prove that for $\mathcal{B}(3)$ this number can be significantly reduced.

Proposition V.1: The Carathéodory's number for the $\mathrm{conv}(\mathcal{U}(3)) = \mathcal{B}(3)$ is 4.

Proof.—Let $B_\infty = \{x \in \mathbb{R}^3 : \|x\|_\infty \le 1\}$ be the unit ball of the infinite norm in $\mathbb{R}^3$, i.e., the cube $[-1,1]^3$. The extreme points of the B_∞ are vertices of the cube, i.e., vectors $v_j = (\pm 1, \pm 1, \pm 1)^T$ for $j = 1, \ldots, 8$. Let $\psi : B_\infty \to \mathbb{M}_{3\times 3}$ be a mapping which sends a vector from the unit ball B_∞ to a diagonal matrix. Then, the ψ sends the extreme points of the B_∞ to the diagonal unitary matrices $U_j = \mathrm{diag}(\pm 1, \pm 1, \pm 1)$ for $j = 1, \ldots, 8$. The Carathéodory's number for the cube is 4. Thus, every point in B_∞ can be written as the convex combination of at most 4 extreme points v_j. In particular every point of the positive octant can be written in this way. This means that every diagonal matrix $D \in \mathbb{M}_{3\times 3}$ with diagonal elements in [0, 1] can be written as convex combination of at most 4 diagonal unitary matrices U_j, i.e., $D = \sum_{i=1}^4 \alpha_i U_i$, with $\alpha_i \ge 0$ and $\sum_{i=1}^4 \alpha_i = 1$. Now, let A be a contraction with a singular value decomposition $A = WDV^\dagger$, where W and V are unitary matrices. This gives

$$A = WDV^\dagger = \sum_{i=1}^4 \alpha_i W U_i V^\dagger. \tag{30}$$

As the $\mathrm{conv}(U(3)) = \mathcal{B}(3)$ is the set of all 3×3 contractions, this completes the proof. ∎

As an immediate consequence of this proposition and the construction used in the proof, *matrices from the* Ω_2 subset, i.e., with two singular values strictly less than one, can be constructed as the convex combination of 3 unitary matrices. Whereas, matrices from the Ω_1 subset, i.e., with only one singular value strictly less than one, can be constructed as the convex combination of two unitary matrices.

Following the idea of Stoer [35], we will show how to construct contractions with two and one singular values strictly less than one as a convex combination of three and two unitary matrices, respectively. Let us take the following diagonal matrix

$$D_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{pmatrix}, \tag{31}$$

where $a, b < 1$. It can be written as the following sum

$$D_1 = \frac{1-a}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{a-b}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{1+b}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{32}$$

Now let us take another diagonal matrix. This time with only one diagonal element strictly less than one

$$D_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & a \end{pmatrix}, \tag{33}$$

where $a < 1$. The D_2 matrix can be written as

$$D_2 = \frac{1-a}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{1+a}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (34)$$

Multiplying D_1 and D_2 matrices from left- and right-hand side by unitary matrices, we end up with a singular value decomposition of a given matrix with singular values gathered in D_1 and D_2, respectively. Moreover a similar construction, where singular values are encoded in the coefficients of the convex combination, can be done for contractions with all three singular values strictly smaller than one. This goes as follows, let

$$D_3 = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}, \quad (35)$$

where a, b, $c < 1$. The D_3 matrix can be written as the following sum

$$D_3 = \frac{1-a}{2}\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{a-b}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{b-c}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{1+c}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (36)$$

Multiplying D_3 by unitary matrices from both sides we get a contraction with singular values a, b, and c.

As a result contractions with three, two and one singular values strictly smaller than one can be written as convex combinations of unitary matrices with singular values encoded in coefficients of the combination. We would also like to highlight that when we multiply the convex combinations D_1, D_2, and D_3 by unitary matrices from both sides we reproduce the relative interiors of the faces of the unit ball in the spectral norm $\mathcal{B}(3)$ introduced in the Theorem IV.2. Thus we have equivalence between these two representations.

These results will be used for extending phenomenological studies on the light-heavy neutrino mixings undertaken in [15] to the $3+2$ and $3+3$ scenarios.

A. Simple example

Let us demonstrate how the above construction can be used for the study of the mixing between active and sterile neutrinos. We will present this for a matrix from the Ω subset, i.e., with two singular values strictly smaller than one, and for the CP invariant scenario. Let us choose the following set of singular values

$$\{\sigma_1 = 1, \sigma_2 = 0.98, \sigma_3 = 0.97\}, \quad (37)$$

which lies within (24). Thus, according to the (31), we can construct the following convex combination

$$D = \frac{1-0.98}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{0.98-0.97}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} + \frac{1+0.97}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (38)$$

To get a physical mixing matrix we have to multiply it by PMNS matrices. For simplicity we will multiply it only from the left-hand side by the following orthogonal matrix

$$O = \begin{pmatrix} 0.831045 & 0.534751 & 0.152986 \\ -0.48083 & 0.552457 & 0.680877 \\ 0.279582 & -0.6394 & 0.716242 \end{pmatrix}, \quad (39)$$

which has been obtained from (7) with the following values of parameters $\theta_{12} = 32.76°$, $\theta_{13} = 8.8°$, $\theta_{23} = 43.55°$. The resulting mixing matrix is

$$T = OD_1 = \begin{pmatrix} 0.831045 & 0.524056 & 0.148396 \\ -0.48083 & 0.541408 & 0.660451 \\ 0.279582 & -0.626612 & 0.694754 \end{pmatrix}, \quad (40)$$

which clearly lies within (7). Alternatively, we can use the equivalence between the relative interiors of the faces of the unit ball $\mathcal{B}(3)$ and the construction in Proposition V.1. In other words the D matrix can be written as a diagonal matrix

$$D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.98 & 0 \\ 0 & 0 & 0.97 \end{pmatrix}, \quad (41)$$

Multiplying it from the left-hand side by the matrix O results in the same matrix T. Thus, we have two equivalent approaches to constructing physical matrices with prescribed singular values.

Information about mixing between active and two sterile neutrinos can be retrieved from the CS decomposition of the 5×5 unitary matrix

$$\begin{pmatrix} U_{\mathrm{PMNS}} & U_{lh} \\ U_{hl} & U_{hh} \end{pmatrix} = \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix} \left(\begin{array}{ccc|cc} 1 & 0 & 0 & 0 & 0 \\ 0 & c_2 & 0 & -s_2 & 0 \\ 0 & 0 & c_3 & 0 & -s_3 \\ \hline 0 & s_2 & 0 & c_2 & 0 \\ 0 & 0 & s_3 & 0 & c_3 \end{array}\right) \begin{pmatrix} Q_1^\dagger & 0 \\ 0 & Q_2^\dagger \end{pmatrix}. \tag{42}$$

From which the submatrix corresponding to the active-sterile mixing reads

$$U_{lh} = W_1 S_{12} Q_2^\dagger, \tag{43}$$

where $W_1 \in \mathbb{C}^{3\times 3}$, $Q_2 \in \mathbb{C}^{2\times 2}$ are unitary matrices (orthogonal matrices in the CP invariant case) and

$$S_{12} = \begin{pmatrix} 0 & 0 \\ -s_2 & 0 \\ 0 & -s_3 \end{pmatrix}. \tag{44}$$

Thus, in the $3+2$ scenario bounds for active-sterile mixing are given by the following formula

$$\begin{aligned} |(U_{lh})_{\alpha j}| &= |w_{\alpha 2} s_1 q_{1j} + w_{\alpha 3} s_2 q_{2j}| \\ &= \left| w_{\alpha 2} q_{1j} \sqrt{1-\sigma_2^2} + w_{\alpha 3} q_{2j} \sqrt{1-\sigma_3^2} \right|, \end{aligned} \tag{45}$$

where $w_{\alpha 2/3}$ are second and third columns of the left singular matrix from the singular value decomposition of the T matrix, which in our case are just columns of the O matrix, and q_{1j}, q_{2j} are elements of the 2×2 orthogonal matrix which is treated as a free parameter. Applying this formula to our case gives

$$\begin{aligned} |(U_{lh})_{e4}| &= |(U_{lh})_{e5}| \le 0.112726, \\ |(U_{lh})_{\mu 4}| &= |(U_{lh})_{\mu 5}| \le 0.198707, \\ |(U_{lh})_{\tau 4}| &= |(U_{lh})_{\tau 5}| \le 0.215658. \end{aligned} \tag{46}$$

The reason that the value of mixing between a given flavor neutrino and the 4th and 5th massive states is the same lies in the fact that in our simplified analysis we focused on the largest possible value which can be obtained and this is the case when q_{1j} and q_{2j} are equal to one. In this way we ignore the fact that sine and cosine in the 2×2 orthogonal matrix Q_2 cannot be simultaneously equal to one. The complete phenomenological analysis of scenarios with 2 and 3 additional sterile neutrinos is much more involving and is beyond the scope of this article. Such complete analysis will be presented in our future work which is still in progress. In general numerical computations with matrices are very sensitive, especially when one is interested in functions of matrix elements such as singular values. The construction of matrices with prescribed singular values is the first step in the simplification of numerical analysis.

We presented two equivalent approaches to the construction of mixing matrices with prescribed singular values, so a cross-check of numerical results in future studies will be possible. The sum representation in Eq. (38) has an advantage over starting directly from Eq. (39) in establishing an entry-wise representation of physical mixing matrices as the singular values are factored out which should simplify relations obtained by the unitary multiplications (work in progress).

VI. VOLUME

Lie groups are also manifolds [39], i.e., they pose geometric structures. Thus, we can associate with them geometrical properties such as the surface area, also called the volume. Two very important groups in physics fall into this category, namely an orthogonal group, and its complex counterpart: a unitary group. These groups are also very important in neutrino physics as the mixing matrix is either orthogonal or, if the CP phase is non-zero, unitary. In Tab. I we gathered the list of structures for which we will calculate the volume in this chapter. The table is split into purely mathematical objects and those restricted by experiments.

A. CP-conserving case

The set of all orthogonal matrices of dimension $n\times n$, i.e., $\mathcal{O}(n) = \{O \in \mathbb{R}^{n\times n} : OO^T = I\}$, is an example of a Stiefel manifold [40]. As the orthogonal matrices have $\frac{n(n-1)}{2}$ independent parameters, the Stiefel manifold of the orthogonal group is a $\frac{n(n-1)}{2}$ dimensional manifold embedded in n^2 space. We can associate to it a volume which is expressed as the Haar measure over the orthogonal group [40–44]

$$\mathrm{vol}(\mathcal{O}(n)) = \int_{\mathcal{O}(n)} [O^T dO]^\wedge, \tag{47}$$

where $[O^T dO]^\wedge$ denotes the wedge product of the matrix $O^T dO$ and dO is the matrix of the differentials of the

TABLE I. Total and experimentally restricted volumes for different structures considered in this work and their mutual relations.

CP-conserving	CP-violating
Total volumes	
$\mathcal{SO}(3) \subset \mathcal{O}(3) \subset \tilde{\mathcal{B}}(3)$	$\mathcal{SU}(3) \subset \mathcal{U}(3) \subset \mathcal{B}(3)$
Experimentally restricted volumes	
$O_{\mathrm{PMNS}} \subset \tilde{\Omega} = \tilde{\mathcal{B}}(3) \cap O_{\mathrm{int}}$	$U_{\mathrm{PMNS}} \subset \Omega = \mathcal{B}(3) \cap U_{\mathrm{int}}$

orthogonal matrix O. This volume can be expressed in the following compact form [44,45]

$$\mathrm{vol}(\mathcal{O}(n)) = \frac{2^n \pi^{\frac{n^2}{2}}}{\Gamma_n(\frac{n}{2})} = \frac{2^n \pi^{\frac{n(n+1)}{4}}}{\prod_{k=1}^{n} \Gamma(\frac{k}{2})}, \tag{48}$$

where $\Gamma_n(x) = \pi^{\frac{n(n-1)}{4}} \Gamma(x)\Gamma(x-\frac{1}{2})\ldots\Gamma(x-\frac{n-1}{2})$. In the case interesting from the neutrino physics perspective, i.e., for $n = 3$, this gives

$$\mathrm{vol}(\mathcal{O}(3)) = 16\pi^2. \tag{49}$$

However, as the determinant of the PMNS mixing matrix is equal to 1, it belongs to even a smaller subset, namely the special orthogonal group $\mathcal{SO}(3)$. The special orthogonal group is a subgroup of $\mathcal{O}(3)$ and its volume is half of the volume of the orthogonal group, i.e.,

$$\mathrm{vol}(\mathcal{SO}(3)) = 8\pi^2. \tag{50}$$

Moreover, the PMNS matrix does not cover the entire range of parameters and hence we must start from $O^T dO$ in order to calculate the volume of this submanifold. Taking the standard PMNS parametrization (7) we get

$$O^T dO = \begin{pmatrix} 0 & d\theta_{12} + s_{13} d\theta_{23} & c_{12} d\theta_{13} - c_{13} s_{12} d\theta_{23} \\ -d\theta_{12} - s_{13} d\theta_{23} & 0 & c_{13} c_{12} d\theta_{23} + s_{12} d\theta_{13} \\ -c_{12} d\theta_{13} + c_{13} s_{12} d\theta_{23} & -c_{13} c_{12} d\theta_{23} - s_{12} d\theta_{13} & 0 \end{pmatrix}. \tag{51}$$

The wedge product of the independent elements of this matrix is equal to

$$[O^T dO]^\wedge = \cos(\theta_{13}) d\theta_{12} d\theta_{13} d\theta_{23}. \tag{52}$$

Thus, the volume of PMNS matrices is given by

$$\mathrm{vol}(\mathrm{PMNS}) = \int_{\theta_{12_L}}^{\theta_{12_U}} \int_{\theta_{13_L}}^{\theta_{13_U}} \int_{\theta_{23_L}}^{\theta_{23_U}} \cos(\theta_{13}) d\theta_{12} d\theta_{13} d\theta_{23}, \tag{53}$$

which with the current experimental limits on θ_{12}, θ_{13}, and θ_{23} (9) gives

$$\mathrm{vol}(\mathrm{PMNS}) = 2.2667 \times 10^{-4}. \tag{54}$$

As we can see the PMNS matrices contribute only in a small portion to the entire $\mathcal{O}(3)$.

B. *CP*-violating case

The unitary group $\mathcal{U}(n)$, i.e., the group of all unitary matrices $\mathcal{U}(n) = \{U \in \mathbb{C}^{n\times n} : UU^\dagger = I\}$, is another example of a Stiefel manifold. Similarly, as for the orthogonal group, the volume of the unitary group is given by the Haar measure over the group

$$\mathrm{vol}(\mathcal{U}(n)) = \int_{U(n)} [U^\dagger dU]^\wedge, \tag{55}$$

where $[U^\dagger dU]^\wedge$ denotes the exterior product of the matrix $U^\dagger dU$ and dU is the matrix of the differentials of the unitary matrix U. The volume of the unitary group can be expressed in a compact form as [41–45]

$$\mathrm{vol}(\mathcal{U}(n)) = \frac{2^n \pi^{n^2}}{\tilde{\Gamma}_n(n)} = \frac{2^n \pi^{\frac{n(n+1)}{2}}}{1!2!\ldots(n-1)!}, \tag{56}$$

where $\tilde{\Gamma}_n(x) = \pi^{\frac{n(n-1)}{2}} \Gamma(x)\Gamma(x-1)\ldots\Gamma(x-n+1)$. Thus, the volume of the 3×3 unitary matrices equals

$$\mathrm{vol}(\mathcal{U}(3)) = 4\pi^6. \tag{57}$$

Moreover, the determinant of the PMNS matrix is equal to one, which means it belongs to the special unitary group $\mathcal{SU}(n)$. The volume of the $\mathcal{SU}(n)$ written in the compact form is [41–43]

$$\mathrm{vol}(\mathcal{SU}(n)) = \frac{2^{\frac{(n-1)}{2}} \pi^{\frac{(n-1)(n+2)}{2}}}{1!2!\ldots(n-1)!}. \tag{58}$$

For the physically interesting dimension, i.e., $n = 3$ this volume is equal to

$$\mathrm{vol}(\mathcal{SU}(3)) = \sqrt{3}\pi^5. \tag{59}$$

The PMNS mixing matrix with nonzero *CP* phase, however, has a restricted set of parameters (5), (6) and ranges of these parameters are confined by experiments (9). Hence, in order to calculate its volume, it is necessary to start from a specific parametrization of the mixing matrix (7). It can be done in the same way as for its real counterpart, i.e., by calculating the wedge product of the matrix $U^\dagger dU$. However, for the complex matrices, it is much more complicated. Alternatively, it can be calculated by determining the Jacobian matrix of the PMNS matrix in the parametrization (7)

$$J = \left(\frac{\partial u_{ij}}{\partial y_k}\right), \quad i,j = 1,\ldots,n \tag{60}$$

and the y_k are parameters (for the PMNS matrix $k = 1,\ldots,4$). Then, the volume element is multiplied by the Jacobian $|J| = \sqrt{\det(\frac{1}{2}J^\dagger J)}$.

The volume of complex PMNS matrices can be calculated in one more way, namely by using the Cartan-Killing metric [46–48]

$$ds^2 = (V,V)dt^2, \tag{61}$$

where $(A,B) = \frac{1}{2}\mathrm{Tr}(A^\dagger B)$ is the inner product induced by the Frobenius norm and $V = U^\dagger dU$. The V is anti-Hermitian and thus $(V,V) = \frac{1}{2}\mathrm{Tr}(V^\dagger V) = -\frac{1}{2}\mathrm{Tr}(V^2)$.

The Hermitian product of the Jacobian matrix for the PMNS matrix is given by

$$\frac{1}{2}J^\dagger J = \begin{pmatrix} 1 & 0 & \sin(\theta_{13})\cos(\delta) & 0 \\ 0 & 1 & 0 & 0 \\ \sin(\theta_{13})\cos(\delta) & 0 & 1 & 0 \\ 0 & 0 & 0 & \sin^2(\theta_{13}) \end{pmatrix}. \tag{62}$$

Let us look also at the expression for the Cartan-Killing metric

$$ds^2 = d\theta_{23}^2 + d\theta_{13}^2 + d\theta_{12}^2 + 2\sin(\theta_{13})\cos(\delta) + \sin^2(\theta_{13})d\delta^2 \tag{63}$$

which as expected gives the same matrix as (62). Finally, the Jacobian for the PMNS matrices is equal to

$$|J| = \sqrt{\sin^2(\theta_{13}) - \cos^2(\delta)\sin^4(\theta_{13})}. \tag{64}$$

Thus, the volume of the complex PMNS matrices is given by

$$\begin{aligned} \mathrm{vol(PMNS)} &= \int_{\mathrm{PMNS}} |J| dV \\ &= \int \sqrt{\sin^2(\theta_{13}) - \cos^2(\delta)\sin^4(\theta_{13})} \\ &\quad \times d\theta_{23} d\theta_{13} d\theta_{12} d\delta. \end{aligned} \tag{65}$$

Taking into account current experimental limits for mixing parameters (9) the numerical value for the volume of the complex PMNS mixing matrices is

$$\mathrm{vol(PMNS)} = 1.4777 \times 10^{-4}. \tag{66}$$

As in the CP conserving case we see that PMNS matrices constitute only a small portion of all unitary matrices.

This and CP invariant result (54) show already the quality of the neutrino studies. However, comparing these results with the volume of quark mixing matrix which is equal to

$$\mathrm{vol(CKM)} = 8.81 \times 10^{-14}, \tag{67}$$

we can see that the quark mixing parameters are much more precise. The CKM mixing matrix can be parametrized in the same way as PMNS in Eq. (7), the exact values of the CKM parameters are taken from [1].

C. Scenarios with extra neutrino states

So far we have established the volume of the neutrino mixing matrices only for the scenario with three known types of neutrinos. However, for scenarios with extra neutrino states, it is required to consider the entire Ω region and not only its extreme points represented by U_{PMNS}. In order to do this, we will use the fact that the region of all physically admissible mixing matrices is a subset of the unit ball in the spectral norm $\mathcal{B}(n) = \{A \in \mathbb{C}^{n\times n} : \|A\| \leq 1\}$ and for the CP conserving case it is restricted to the real matrices $\tilde{\mathcal{B}}(n) = \{A \in \mathbb{R}^{n\times n} : \|A\| \leq 1\}$. Volumes of the $\mathcal{B}(n)$ and $\tilde{\mathcal{B}}(n)$ can be calculated from the singular value decomposition. The differential of the singular value decomposition of a given matrix $A = U\Sigma V^\dagger$ is equal to

$$dA = dU\Sigma V^\dagger + Ud\Sigma V^\dagger + U\Sigma dV^\dagger. \tag{68}$$

By multiplying this from the left-hand side by $U^\dagger$ and from the right-hand side by V we get

$$dX \equiv U^\dagger dAV = U^\dagger dU\Sigma + d\Sigma + \Sigma dV^\dagger V, \tag{69}$$

which can be rewritten using $dV^\dagger V = -V^\dagger dV$ in the following form

$$dX = U^\dagger dAV = U^\dagger dU\Sigma + d\Sigma - \Sigma V^\dagger dV. \tag{70}$$

The Haar measure is left- and right-invariant, thus $[dA]^\wedge = [U^\dagger dAV]^\wedge = [dX]^\wedge$. The entrywise analysis of the dX in the CP invariant scenario gives

$$[dX]^\wedge = \prod_{i<j} |\sigma_j^2 - \sigma_i^2| \wedge_{i=1}^n d\sigma_i [O^T dO]^\wedge [Q^T dQ]^\wedge. \tag{71}$$

Hence, the volume of the unit ball of the spectral norm in a real case is given by

$$\mathrm{vol}(\tilde{\mathcal{B}}(n)) = \frac{1}{2^n n!}\mathrm{vol}(\mathcal{O}(n))^2 \int_0^1 \prod_{i<j} |\sigma_j^2 - \sigma_i^2| \prod_{k=1}^n d\sigma_k. \tag{72}$$

The inclusion of the factor $\frac{1}{2^n}$ assures the uniqueness of the singular value decomposition. For the physically interesting dimension $n = 3$, we have

$$\mathrm{vol}(\tilde{\mathcal{B}}(3)) = \frac{8\pi^4}{45}. \tag{73}$$

Similar entrywise analysis of the (70) provides the volume element for the singular value decomposition of complex matrices

$$[dX]^\wedge = \prod_{i=1}^{n} \sigma_i \prod_{i<j} |\sigma_j^2 - \sigma_i^2|^2 \wedge_{i=1}^{n} d\sigma_i [U^\dagger dU]^\wedge [V^\dagger dV]^\wedge. \tag{74}$$

Thus, the volume of the unit ball of the spectral norm is given by

$$\mathrm{vol}(\mathcal{B}(n)) = \frac{1}{(2\pi)^n n!} \mathrm{vol}(\mathcal{U}(n))^2 \times \int_0^1 \prod_{k=1}^{n} \sigma_k \prod_{i<j} |\sigma_j^2 - \sigma_i^2|^2 \prod_{k=1}^{n} d\sigma_k. \tag{75}$$

The factor $\frac{1}{(2\pi)^n}$ ensures the uniqueness of the singular value decomposition. In the case interesting from the neutrino physics perspective, i.e., $n = 3$, this gives

$$\mathrm{vol}(\mathcal{B}(3)) = \frac{\pi^9}{8640}. \tag{76}$$

We can use the formulas for the volumes of $\mathcal{B}(3)$ and $\tilde{\mathcal{B}}(3)$ as the basis in the calculation of the volume of the Ω region. As the Ω region is defined as the convex hull of the PMNS matrices, to find its volume we need to replace in the formulas (72) and (75) $\mathrm{vol}(\mathcal{U}(n))$ and $\mathrm{vol}(\mathcal{O}(n))$ by vol (PMNS) in the general and CP conserving case, respectively. Moreover, it is also necessary to restrict ranges of singular values for those allowed by current experimental data (24). As the result, for the CP invariant scenario, we have the following formula

$$\mathrm{vol}(\tilde{\Omega}) = \frac{1}{2^n n!} \mathrm{vol}(\mathrm{PMNS})^2 \int_{\sigma_{\min}}^{1} \prod_{i<j} |\sigma_j^2 - \sigma_i^2| \prod_{k=1}^{n} d\sigma_k. \tag{77}$$

Taking into account current experimental bounds (9) and allowed ranges for singular values (24), the numerical value is equal

$$\mathrm{vol}(\tilde{\Omega}) = 6.45 \times 10^{-16}. \tag{78}$$

Thus, the Ω region in the CP invariant case constitutes only 3.72×10^{-17} of the unit ball (72).

For the general case including the CP phase, the formula for the volume of the Ω region is given by

$$\mathrm{vol}(\Omega) = \frac{1}{(2\pi)^n n!} \mathrm{vol}(\mathrm{PMNS})^2 \times \int_{\sigma_{\min}}^{1} \prod_{k=1}^{n} \sigma_k \prod_{i<j} |\sigma_j^2 - \sigma_i^2|^2 \prod_{k=1}^{n} d\sigma_k, \tag{79}$$

and its numerical value is

$$\mathrm{vol}(\Omega) = 1.12 \times 10^{-18}. \tag{80}$$

In the complex case, the contribution of the Ω region is even smaller than in the CP invariant scenario and it constitutes only 3.24×10^{-19} of the respective unit ball in the spectral norm (75). It may look like that $\mathrm{vol}(\tilde{\Omega})$ is larger than the $\mathrm{vol}(\Omega)$, however, we must keep in mind that $\tilde{\Omega}$ and Ω are structures of different dimensions, and thus cannot be compared directly. Let us also calculate the volume of the physical region for the quark sector. It is given by the same formula as for $\mathrm{vol}(\Omega)$, but lower limit of singular values are now much closer to one $\{\sigma_1 = 0.99997, \sigma_2 = 99965, \sigma_3 = 0.99890\}$

$$\mathrm{vol}(\Omega_{\mathrm{CKM}}) = 1.95 \times 10^{-59}. \tag{81}$$

This once again emphasizes the difference of precision in data between neutrino and quark sectors.

We have established earlier the characterization of the Ω region as the intersection of the $\mathcal{B}(3)$ and U_{int} (20). The U_{int} can be treated as a hyperrectangle in $\mathbb{R}^9$ or $\mathbb{C}^9 \simeq \mathbb{R}^{18}$ respectively for the CP invariant case and the general case. As such, they also are geometric structures with associated volume. This volume is simply the product of the length of its sides, i.e., given intervals. Thus for the CP conserving case, it gives

$$\mathrm{vol}(O_{\mathrm{int}}) = 2.84 \times 10^{-10}. \tag{82}$$

Whereas when the CP phase is taken into account it is equal to

$$\mathrm{vol}(U_{\mathrm{int}}) = 2.27 \times 10^{-11}. \tag{83}$$

In [14] statistical analysis was performed concerning the amount of physically admissible mixing matrices contained within the interval matrix U_{int}. The analysis establishes that for the CP invariant scenario only about 4% of matrices within the interval matrix are contractions. Comparison of volumes gives a similar qualitative result, namely contractions make a small part of the U_{int}. The exact calculation reveals that the volume of the Ω region constitutes 2.3×10^{-4}

percent of $O_{\rm int}$ in the CP conserving case and 8.12×10^{-6} percent of $U_{\rm int}$ for the general complex scenario.

We can check how vol(Ω) and vol(PMNS) are sensitive to the precision of neutrino parameters. For example, if the range of the CP phase shrinks twice, i.e., we assume $\delta \in [182.5°, 306°]$ then we get

$$\begin{aligned} \text{vol(PMNS)} &= 7.345 \times 10^{-5}, \\ \text{vol}(\Omega) &= 2.759 \times 10^{-19}. \end{aligned} \tag{84}$$

We can see that vol (PMNS) decreased twice, however, its value is still a few orders of magnitudes higher than for vol (CKM), while vol(Ω) decreased almost by order of magnitude.

Using the notion of the volume we can try to quantify the difference between unitary (SM) and nonunitary (BSM) mixing matrices. First, we take the ratio of the volume of unitary PMNS mixing matrices vol (PMNS) and the volume of the region of physical mixing matrices vol(Ω)

$$\mathcal{R} = \frac{\text{vol}(\Omega)}{\text{vol(PMNS)}}, \qquad \mathcal{R} \in [0, 1]. \tag{85}$$

We get for general and CP invariant neutrino scenarios as well as for the quark sector the following estimates

$$\begin{aligned} \mathcal{R} &= \frac{\text{vol}(\Omega)}{\text{vol(PMNS)}} = \frac{1.12 \times 10^{-18}}{1.4777 \times 10^{-4}} = 7.57935 \times 10^{-15}, \\ \tilde{\mathcal{R}} &= \frac{\text{vol}(\tilde{\Omega})}{\text{vol(PMNS)}} = \frac{6.45 \times 10^{-16}}{2.2667 \times 10^{-4}} = 2.84555 \times 10^{-12}, \\ \mathcal{R}_{\rm CKM} &= \frac{\text{vol}(\Omega_{CKM)}}{\text{vol}(CKM)} = \frac{1.95 \times 10^{-59}}{8.81 \times 10^{-14}} = 2.21339 \times 10^{-46}. \end{aligned} \tag{86}$$

The above R ratios go to zero when we approach unitarity (vol(Ω) tends to zero in this case).

Second, we use a properly normalized difference of vol(Ω) and vol (PMNS). The volume of unitary matrices will be normalized to one whereas the volume of the Ω will be normalized by $a * \text{vol(PMNS)}^2 * I_{\mathcal{B}(3)}$, where $a = \frac{1}{(2\pi)^n n!}$ or $\tilde{a} = \frac{1}{2^n n!}$ in the CP invariant case and $I_{\mathcal{B}(3)} = \int_0^1 \prod_{k=1}^n \sigma_k \prod_{i<j} |\sigma_j^2 - \sigma_i^2|^2 \prod_{k=1}^n d\sigma_k$ or $I_{\tilde{\mathcal{B}}(3)} = \int_0^1 \prod_{i<j} |\sigma_j^2 - \sigma_i^2| \prod_{k=1}^n d\sigma_k$ in the case of CP invariance. Hence we use the ratio of respective integrals of vol(Ω) and vol($\mathcal{B}(3)$), respectively. This ensures that both quantities are dimensionless and we can subtract them. Thus, we are interested in the following quantity

$$\mathcal{D} = 1 - \frac{\text{vol}(\Omega)}{a * \text{vol(PMNS)}^2 * I_{\mathcal{B}(3)}} = 1 - \frac{I_\Omega}{I_{\mathcal{B}(3)}}. \tag{87}$$

In this way we measure deviation from the SM in terms of volumes. The results are

$$\begin{aligned} \mathcal{D} &= 1 - 2.19 \times 10^{-4} = 0.999781, \\ \tilde{\mathcal{D}} &= 1 - 1.8 \times 10^{-5} = 0.999982, \\ \mathcal{D}_{\rm CKM} &= 1 - 1.077 \times 10^{-26}. \end{aligned} \tag{88}$$

These results show that the quark mixing matrix is almost unitary, whereas in the case of neutrinos the mixing matrix is much closer to being unitary in the CP invariant scenario than for the general case, which shows that the experimental determination of the CP phase δ still requires much improvement.

VII. SUMMARY AND OUTLOOK

Neutrino mixings between the three known active neutrino states can be described by a 3×3 matrix which is unitary. In the case of hypothetical extra neutrino species the 3×3 mixing matrix must be extended to a larger unitary matrix.

In general, the physical space of neutrino mixings determined experimentally constitutes a geometric region of finite convex combinations of unitary 3×3 PMNS mixing matrices. We studied the structure of this region, which is a part of a unit ball of a spectral norm.

We have described subsets corresponding to a different minimal number of additional neutrinos as relative interiors of faces of this unit ball. This feature of the geometric region allows for the independent phenomenological analysis of $3 + n$ neutrino mixing models. We also gave an alternative characteristic of these subsets in terms of Ky-Fan k-norms.

We showed that the Carathéodory's number for the Ω region equals maximally four. In $3 + 1$ and $3 + 2$ scenarios, the Carathéodory's number is 2 and 3, respectively. This result allows constructing all matrices from the region as the convex combination in an optimal way. We demonstrated a particular construction of contractions with one, two and three singular values strictly less than one, and with singular values encoded in the coefficients. Knowing the basis with a minimal number of generating matrices, we will be able to make concrete phenomenological studies of light-heavy neutrino mixings *independently* in $3 + 2$ and $3 + 3$ scenarios. It will extend our previous studies using the dilation procedure and obtained limits on active-sterile mixings in the $3 + 1$ scenario where one extra neutrino state is present [15].

We established the size of the region of the physically admissible mixing matrices by calculating its volume. As zero volume would mean that neutrino parameters are determined experimentally without errors, its size informs us in some way about the fidelity of experimental data extraction. In the case of three neutrino mixing scenario this volume shows that in neutrino physics, compared to the whole space of the mixing parameters, a space of possible neutrino mixing parameters is already restricted considerably,

though when comparing with quark mixings and corresponding volume, the neutrino volume is many orders of magnitude larger. When additional neutrinos are under consideration the region narrows down comparing to $\mathcal{B}(3)$ and U_{int} where $\mathcal{B}(3)$ describes all 3×3 contractions whereas U_{int} contains experimentally established ranges for neutrino mixing matrices and Ω is the intersection of these two structures. The size of this region will be further squeezed by the increasing precision (via increasing statistics) of future neutrino physics experiments, especially for CP-violating scenarios when the Dirac CP-phase will be determined.

As an outlook, apart from studying unitary extensions of admissible matrices from the Ω region and the light-heavy neutrino mixings, we also plan to apply methods of semidefinite programming and find information about the position of the Ω region within the unit ball of the spectral norm. This study will help determine the prefered parameter space for future searches for sterile neutrinos in models with different number of extra neutrino states.

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APPENDIX A: NORMS

Definition 8: A matrix norm is a function $\|\cdot\|$ from the set of all matrices $\mathbb{M}_{n\times m}$ into $\mathbb{R}$ that satisfies the following properties

$$\begin{aligned}&\|A\| \geq 0 \quad \text{and} \quad \|A\| = 0 \Leftrightarrow A = 0,\\ &\|\alpha A\| = |\alpha|\|A\|,\\ &\|A + B\| \leq \|A\| + \|B\|,\\ &\|AB\| \leq \|A\|\|B\|.\end{aligned} \tag{A1}$$

In other words, the matrix norm is a vector norm with the additional condition of submultiplicativity.

There exists an important class of matrix norms consisting of matrix norms which do not change by the unitary multiplication.

Definition 9: A matrix norm $\|\cdot\|$ is called unitarily invariant if for every unitary matrices U, V and a given matrix A it satisfies

$$\|UAV\| = \|A\|. \tag{A2}$$

Another important class of matrix norms, called the induced matrix norms, contains matrix norms that are obtained from the vector norms in the following way

$$\|A\|_\star = \max_{\|x\|_\star = 1} \|Ax\|_\star, \tag{A3}$$

where $\|\cdot\|_\star$ stands for the corresponding vector norm. In our case, of particular interest is the matrix norm induced from the Euclidean 2-norm $\|x\|_2 = \sqrt{\sum_{i=1}^n x_i^2} = \sqrt{(x,x)} = \sqrt{x^\dagger x}$ for $x = (x_1, \ldots, x_n)^T$. From the Rayleigh quotient $\lambda_{\max}(A) = \max_{\|x\|_2=1} x^\dagger A x$ [49], we have

$$\begin{aligned}\|A\|_2^2 &= \max_{\|x\|_2=1} \|Ax\|_2^2 = \max_{\|x\|_2=1} (Ax)^\dagger Ax = \max_{\|x\|_2=1} x^\dagger A^\dagger A x\\ &= \lambda_{\max}(A^\dagger A) = \sigma_1^2(A).\end{aligned} \tag{A4}$$

Thus, the matrix norm $\|\cdot\|_2$ can be defined as the largest singular value of a given matrix. This matrix norm is called an operator norm or spectral norm and will be denoted as $\|\cdot\|$. Thus,

Definition 10: A spectral norm of a matrix $A \in \mathbb{M}_{n\times m}$ is the matrix norm defined as

$$\|A\| = \max_{\|x\|_2=1} \|Ax\|_2 = \sigma_1(A). \tag{A5}$$

Moreover, the spectral norm is also a unitary invariant norm (A2).

APPENDIX B: COSINE-SINE (CS) DECOMPOSITION

Theorem B.1: Let the unitary matrix $U \in \mathbb{M}_{(n+m)\times(n+m)}$ be partitioned as

$$U = \begin{array}{c} \\ n \\ m \end{array} \begin{array}{c} \begin{array}{cc} n & m \end{array} \\ \begin{pmatrix} U_{\text{PMNS}} & U_{lh} \\ U_{hl} & U_{hh} \end{pmatrix} \end{array}, \tag{B1}$$

If $m \geq n$, then there are unitary matrices $W_1, Q_1 \in M_{n\times n}$ and unitary matrices $W_2, Q_2 \in \mathbb{M}_{m\times m}$ such that

$$\begin{aligned}&\begin{pmatrix} U_{\text{PMNS}} & U_{lh} \\ U_{hl} & U_{hh} \end{pmatrix}\\ &= \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix} \left(\begin{array}{c|cc} C & -S & 0 \\ \hline S & C & 0 \\ 0 & 0 & I_{m-n} \end{array}\right) \begin{pmatrix} Q_1^\dagger & 0 \\ 0 & Q_2^\dagger \end{pmatrix},\end{aligned} \tag{B2}$$

where $C \geq 0$ and $S \geq 0$ are diagonal matrices satisfying $C^2 + S^2 = I_n$.

There exists another form of the CS decomposition which is more important from the neutrino physics perspective. Let U_{PMNS} have the singular value decomposition $U_{\text{PMNS}} = W_1 \text{diag}(I_r, C) Q_1^\dagger$, where I_r denotes r singular values equal to one, and C contains singular values that are strictly less than one. The structure of the CS decomposition reveals the intriguing fact, namely the minimal dimension of the unitary dilation of a given contraction is not arbitrary, but is encoded in the number of singular values strictly less than one.

Corollary 1: The parametrization of the unitary dilation of the smallest size is given by

$$\begin{pmatrix} U_{\mathrm{PMNS}} & U_{lh} \\ U_{hl} & U_{hh} \end{pmatrix} = \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix} \left(\begin{array}{cc|c} I_r & 0 & 0 \\ 0 & C & -S \\ \hline 0 & S & C \end{array}\right) \times \begin{pmatrix} Q_1^\dagger & 0 \\ 0 & Q_2^\dagger \end{pmatrix}, \tag{B3}$$

where $r = n - m$ is the number of singular values equal to 1 and $C = \mathrm{diag}(\cos\theta_1, \ldots, \cos\theta_m)$ with $|\cos\theta_i| < 1$ for $i = 1, \ldots, m$.

This is crucial from the physical point of view, since it tells that the minimal number of sterile neutrinos is not arbitrary, but depends on the singular values of the PMNS mixing matrix.

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