Unitarity and the three flavor neutrino mixing matrix

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Unitarity is a fundamental property of any theory required to ensure we work in a theoretically consistent framework. In comparison with the quark sector, experimental tests of unitarity for the 3×3 neutrino mixing matrix are considerably weaker. We perform a reanalysis to see how global knowledge is altered when one refits oscillation results without assuming unitarity, and present 3σ ranges for allowed U_{PMNS} elements consistent with all observed phenomena. We calculate, for the first time, bounds on the closure of the six neutrino unitarity triangles, with the closure of the $\nu_e\nu_\mu$ triangle being constrained to be ≤ 0.03, while the remaining triangles are significantly less constrained to be ≤ 0.1–0.2. Similarly for the row and column normalization, we find their deviation from unity is constrained to be ≤ 0.2–0.4, for four out of six such normalizations, while for the ν_μ and ν_e row normalization the deviations are constrained to be ≤ 0.07, all at the 3σ CL. We emphasize that there is significant room for new low energy physics, especially in the ν_τ sector which very few current experiments constrain directly.

With the knowledge of $\sin^2 2\theta_{13}$ now almost at the 5% level, and interplay between the long baseline accelerator $\nu_\mu \to \nu_e$ appearance data [1,2] and short baseline reactor $\bar{\nu}_e \to \bar{\nu}_e$ disappearance [3–5] data, combined with prior knowledge of θ_{23} from $\nu_\mu \to \nu_\mu$ disappearance data [6–8], suggesting tentative global hints at $\delta_{CP} \approx 3\pi/2$, there is much merit to statements that we are now in the precision measurement era of neutrino physics.

Our knowledge of the distinct Pontecorvo-Maki-Nakagawa-Sakata (PMNS) neutrino mixing matrix elements comes from the plethora of successful experiments that have run since the first strong evidence for neutrino oscillations, interpreted as $\nu_\mu \to \nu_\tau$ oscillations, was discovered by Super-Kamiokande in 1998 [9]. However, one must always remember that our knowledge of the matrix elements comes predominantly from high statistics $\bar{\nu}_e$ disappearance and ν_μ disappearance experiments, with the concept of unitarity being invoked to disseminate this information onto the remaining elements.

Unitarity of a mixing matrix is a necessary condition for a theoretically consistent description of the underlying physics, as nonunitarity directly corresponds to a violation of probability in the calculated amplitudes. In the neutrino sector unitarity can be directly verified by precise measurement of each of the mixing elements to confirm the unitarity condition: $U^\dagger U = \mathbb{1} = UU^\dagger$. In this there are 12 conditions, six of which we will refer to as normalizations (sum of the squares of each row or column, e.g. the ν_e normalization $|U_{e1}|^2 + |U_{e2}|^2 + |U_{e3}|^2 = 1$) and six conditions that measure the degree to which each unitarity triangle closes (e.g. the $\nu_e\nu_\mu$ triangle: $U_{e1}U_{\mu 1}^* + U_{e2}U_{\mu 2}^* + U_{e3}U_{\mu 3}^* = 0$). See Qian *et al.* [10]

for a detailed discussion of the current and future state of measurements of the ν_e normalization.

In the quark sector, the analogous situation involving the Cabibbo-Kobayashi-Maskawa (CKM) matrix has been subject to intense verification as many experiments have access to all of the V_{CKM} elements individually. Current data show that the assumption of unitarity for the 3×3 CKM matrix is valid in the quark sector to a high precision, with the strongest normalization constraint being $|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9999 \pm 0.0006$ and the weakest still being significant at $|V_{ub}|^2 + |V_{cb}|^2 + |V_{tb}|^2 = 1.044 \pm 0.06$ [11]. Unlike the quark sector, however, experimental tests of unitarity are considerably weaker in the 3×3 U_{PMNS} neutrino mixing matrix. It remains an initial theoretical assumption inherent in many analyses [12–14], but is the basis for the validity of the 3ν paradigm.

This nonunitarity can arise naturally in a large variety of theories. A generic feature of many beyond the Standard Model scenarios is the inclusion of one or more new massive fermionic singlets, uncharged under the Standard Model (SM) gauge group, $SU(3)_C \times SU(2)_L \times U(1)_Y$. If these new states mix with the SM neutrinos then the true mixing matrix is enlarged from the 3×3 U_{PMNS} matrix to an $n \times n$ matrix,

$$
U_{\text{PMNS}}^{\text{Extended}} = \begin{pmatrix} \overbrace{\begin{pmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3} \\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3} \end{pmatrix}}^{U_{\text{PMNS}}^{3\times 3}} & \cdots & U_{en} \\ & \cdots & U_{\mu n} \\ & \cdots & U_{\tau n} \\ \vdots \quad \vdots \quad \vdots & \ddots & \vdots \\ U_{s_n 1} \quad U_{s_n 2} \quad U_{s_n 3} & \cdots & U_{s_n n} \end{pmatrix}.
$$

These so-called sterile neutrinos have been a major discussion point for both the theoretical and experimental communities for decades. *A priori* these new states can sit at practically any mass as there is no known symmetry to dictate a scale. Although this extended $n \times n$ mixing matrix, should nature choose it, will indeed be unitary to preserve probability, the same is not true for any given $m \times m$ subset, with $m < n$. This is the canonical model of how new physics, introduced at any scale, breaks observed unitarity in the neutrino sector.

If this physics enters solely at a high scale, as in the minimal unitarity violation (MUV) scheme [15], then one can utilize weak decays, rare lepton decays (e.g. $\mu \to e\gamma$) and electroweak (EW) precision measurements to bound the amount of nonunitarity to the level of 0.5% [16].

Here we consider the alternative case in which the new physics that provides this nonunitarity enters at a relatively low scale, as several current experimental hints suggest with anomalous results from LSND [17], MiniBooNE [18], the gallium anomaly [19,20] and the reactor anomaly [21]. In this regime neutrino oscillations are the most important experimental probe we have access to. The most convincing means of verification of unitarity in the neutrino sector would be analogous to the quark sector, via direct and independent measurement of all the U_{PMNS} elements, to overconstrain the parameter space and confirm that the 12 unitarity constraints hold to within experimental precision. However, we do not currently have access to enough experiments in the ν_μ and ν_τ sectors to bound all of the elements to a sufficient degree to verify all 12 conditions. Thus we must look for alternative ways to constrain the U_{PMNS} elements.

One can perform indirect searches of unitarity by searching for mixing elements outside those of the 3ν mixing regime. These classes of searches do not measure the 3×3 mixing elements *per se*, but rather by looking for additional states one can constrain the violations they would induce in the 3×3 subset. One proceeds by noting all null results at frequencies distinct to those of the 3ν paradigm. We do not wish to perform a global fit for new physics as this has been well covered in the literature [22,23]. Instead we focus on what unresolved physics can do to our current precision; hence we do not include any positive signals such as LSND or the MiniBooNE anomaly.

Such a sterile driven approach requires additional assumptions on the exact origin of the nonunitarity, thus losing some model independence. However, as an extended U_{PMNS} matrix encompasses many beyond the Standard Model scenarios, it is natural to include this in our analysis. To proceed one must then consider what scale the new physics enters at; however, as we do not focus on the origin of such nonunitarity we choose to marginalize over the new scale(s) assuming the possibility that they enter in at an oscillating scale, with at least $|\Delta m^2| \geq 10^{-2}$ eV^2. Below this scale, states that degenerate with SM neutrinos require a much more detailed analysis.

A nonunitary mixing matrix can be parametrized as a 3×3 matrix hosting 9 complex nonunitary elements, 5 phases of which can be removed by rephasing the lepton fields, leaving 13 parameters: 9 real positive numbers and 4 phases. There are many ways to parametrize this matrix, e.g. [24]; however for clarity we choose to keep it directly in terms of its matrix elements. The oscillation probability for a neutrino (antineutrino) of initial flavor α and energy E_ν to transition to a neutrino (antineutrino) of flavor β after a distance L with such a nonunitary mixing matrix is given by

$$P\left(\overset{(-)}{\nu_\alpha} \to \overset{(-)}{\nu_\beta}\right) = \left|\sum_{i=1} U_{\beta i}^* U_{\alpha i}\right|^2$$

$$-4\sum_{i<j} \Re(U_{\beta i} U_{\beta j}^* U_{\alpha i} U_{\alpha j}^*) \sin^2\left(\Delta m_{ji}^2 \frac{L}{4E_\nu}\right)$$

$$\overset{(-)}{+} 2\sum_{i<j} \Im(U_{\beta i} U_{\beta j}^* U_{\alpha i} U_{\alpha j}^*) \sin\left(\Delta m_{ji}^2 \frac{L}{2E_\nu}\right),$$

where now, without assuming unitarity, the leading term is not a function of $\Delta m^2 L/E_\nu$ and is also not necessarily equal to 1 or 0 in neutrino disappearance and appearance experiments respectively.

Although violations of unitarity such as these modify the oscillation amplitudes and total normalization of the probability, they do not have any effect on the oscillation frequency, which remains a function of the mass differences and L/E_ν only (ignoring higher order nonunitary matter effects). Thus, for simplicity of analysis the global best fit values for the mass squared differences are assumed ($\Delta m_{21}^2 = 7.6 \times 10^{-5}$ eV^2, $|\Delta m_{31}^2| = 2.4 \times 10^{-3}$ eV^2) [11].

For each observed oscillation one can then directly compare the measured amplitude with the nonunitary expression for the oscillation probability. It is this amplitude matching that we use to undertake a global fit and that provides us the ranges for U_{PMNS} that would successfully reproduce the measured oscillation amplitudes and normalizations. We focus on the physically motivated subclass of unitarity violations such that $|U_{\alpha 1}|^2 + |U_{\alpha 2}|^2 + |U_{\alpha 3}|^2 \leq 1$, for $\alpha = e, \mu, \tau$, and $|U_{ei}|^2 + |U_{\mu i}|^2 + |U_{\tau i}|^2 \leq 1$ for $i = 1, 2, 3$. One must also use the knowledge of the unitarity of the true extended mixing matrix to invoke Cauchy-Schwartz inequalities and place six geometric constraints on the mixing elements [15],

$$\left|\sum_{i=1}^3 U_{\alpha i} U_{\beta i}^*\right|^2 \leq \left(1 - \sum_{i=1}^3 |U_{\alpha i}|^2\right)\left(1 - \sum_{i=1}^3 |U_{\beta i}|^2\right),$$

$$\text{for } \alpha, \beta = (e, \mu, \tau), \qquad \alpha \neq \beta,$$

$$\left|\sum_{\alpha=e}^\tau U_{\alpha i} U_{\alpha j}^*\right|^2 \leq \left(1 - \sum_{\alpha=e}^\tau |U_{\alpha i}|^2\right)\left(1 - \sum_{\alpha=e}^\tau |U_{\alpha j}|^2\right),$$

$$\text{for } i, j = (1, 2, 3), \qquad i \neq j.$$

These Cauchy-Schwartz constraints enable precision measurements in a single sector to be passed subsequently to all elements of the mixing matrix [25].

To perform the analysis, for each experiment considered [26] we take the observed amplitude of the $\nu_\alpha \to \nu_\beta$ (or $\bar{\nu}_\alpha \to \bar{\nu}_\beta$) oscillation alongside its published uncertainty and construct a chi-squared for the associated nonunitary amplitudes, along with any necessary normalization systematics as pull factors. For short-baseline (SBL) sterile searches, if an experiment publishes the resultant χ^2 surface of their analyses in a $3+N$ format then this is used as a prior to bound any nonunitarity. Otherwise an appropriate prior is estimated by performing a $3+N$ fit to published data.

We minimize the constructed χ^2 over all parameters, satisfying the Cauchy-Schwartz constraints, using a Markov chain Monte Carlo minimizer. The results of the analyses are shown in Fig. 1, without unitarity (red solid line) and with the assumption of unitarity (black dashed line). The nonunitary analysis was performed under the strict assumption that any nonunitarity comes solely from an extended $U_{\rm PMNS}$ and that no new interactions, such as an additional $U(1)'$ which can lead to strongly modified matter effects, are active at oscillation energies [62].

Upon minimization the best fit points agree in both unitary and nonunitary fits. To compare how the precision varies we consider the frequentist 3σ ranges of the one-dimensional $\Delta\chi^2$ projections without unitarity assumed (with unitarity), where we marginalize over all parameters except the one in question, we obtain

$$
|U|_{3\sigma}^{\substack{\text{w/o Unitarity} \\ \text{(with Unitarity)}}} = \begin{pmatrix} \underset{(0.79\to0.85)}{0.76 \to 0.85} & \underset{(0.50\to0.59)}{0.50 \to 0.60} & \underset{(0.14\to0.16)}{0.13 \to 0.16} \\ \underset{(0.22\to0.52)}{0.21 \to 0.54} & \underset{(0.43\to0.70)}{0.42 \to 0.70} & \underset{(0.62\to0.79)}{0.61 \to 0.79} \\ \underset{(0.24\to0.54)}{0.18 \to 0.58} & \underset{(0.47\to0.72)}{0.38 \to 0.72} & \underset{(0.60\to0.77)}{(0.40 \to 0.78)} \end{pmatrix}.
$$

The ranges for the individual elements, assuming unitarity (bracketed numbers in above expression), are in good agreement with published results in contemporary global fits such as ν-fit [12].

If we define the shift in the range of allowed values as the ratio of the difference in 3σ ranges without and with unitarity to the range derived solely with unitarity, the increases in parameter space for $|U_{ei}|, i = 2, 3$ and $|U_{\mu i}|, i = 1, 2, 3$ are all $\leq 10\%$ (4%, 8%, 8%, 7% and 4%
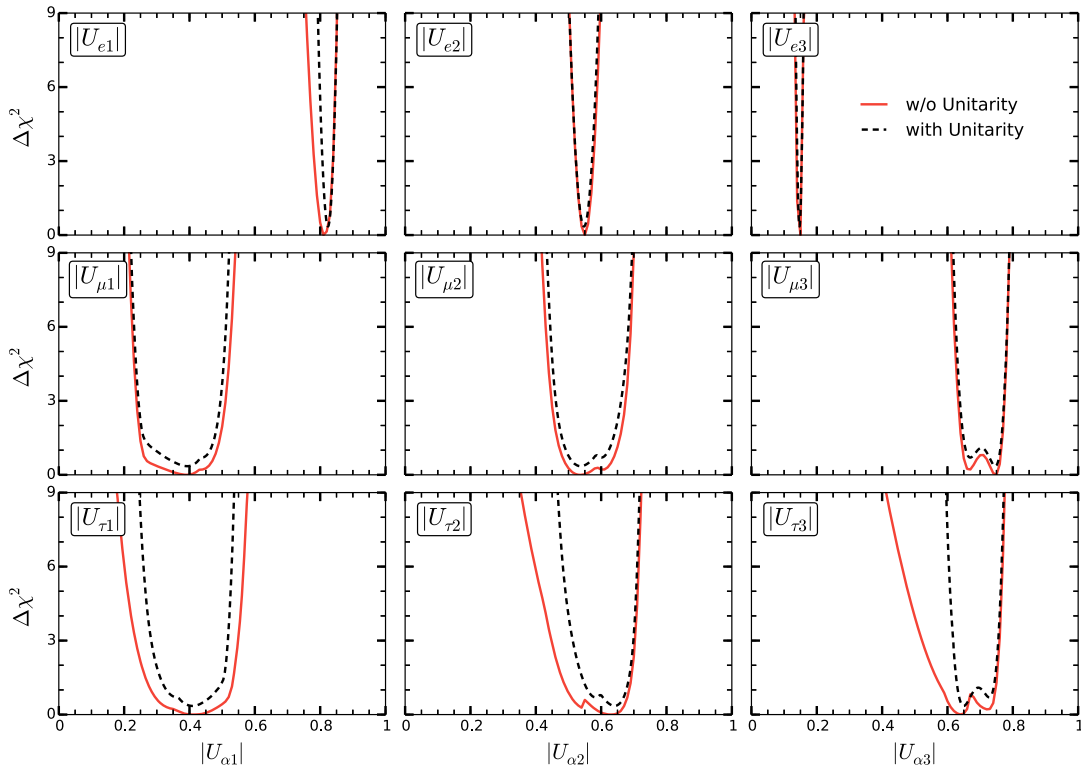

FIG. 1.   Marginalized 1-D $\Delta\chi^2$ for each of the magnitudes of the 3×3 neutrino mixing matrix elements, without (red solid) and with (black dashed) the assumption of unitarity. The x-axis is the magnitude of each individual matrix element, and the y-axis is the associated $\Delta\chi^2$ after marginalization over all parameters other than the one in question. This analysis was performed for the normal hierarchy, the inverse hierarchy providing the same qualitative result.

respectively), with $|U_{e1}|$ taking the majority of the discrepancy in the ν_e sector, with an increase of allowed range of 68%, primarily due to the weaker bounds from KamLAND compared to the SBL reactors. The entire ν_τ sector, however, may contain substantial discrepancies from unitarity with shifts in allowed regions of 37%, 46% and 104% respectively.

We must stress that even if the 3σ ranges of the U_{PMNS} elements agree closely with the unitarity case, this does not equate to the neutrino mixing matrix being unitary. In the unitary case the correlations are much stronger and choosing an exact value for any one the mixing elements drastically reduces the uncertainty on the remaining elements. One can address this issue by looking at the row and column unitarity triangle closures and the row and column normalizations to better understand the level at which we know unitarity is violated or not.

For the case of the six neutrino unitarity triangles, we present, for the first time, the allowed ranges for their closures in Fig. 2. For the three row unitarity triangles the bounds originate from a combination of the corresponding Cauchy-Schwartz inequalities along with appearance data in the respective channel. The column unitarity triangles, being bound primarily by the geometric constraints and not direct measurement, are less known. Only one unitarity triangle does not contain a ν_τ element, the $\nu_e\nu_\mu$ unitarity triangle, and hence it is the only unitarity triangle in which it is constrained to be closed by ≤ 0.03 at the 3σ CL, compared to ≤ 0.1–0.2 at the 3σ CL for the remaining unitarity triangles. This hierarchical situation will not improve unless precise measurements can be made in

FIG. 3. 1-D $\Delta\chi^2$ for deviation of both U_{PMNS} row (solid) and column (dashed) normalizations, when considering new physics that enters above $|\Delta m^2| \geq 10^{-2}$ eV^2.

the ν_τ sector. We also plot the resultant ranges for the normalizations in Fig 3. We see that the ν_e and ν_μ normalization deviations from unity are relatively well constrained (≤ 0.06 and 0.07 at 3σ CL respectively), primarily by reactor fluxes and a combination of precision measurements of the rate and spectra of upward-going muonlike events observed at Super-Kamiokande [27]. We note the ν_μ normalization deviation from unity is constrained slightly ($\approx 1\%$) better than the ν_e normalization. This is due to the large theoretical error, 5%, on total flux from reactors assumed [28]. The remaining normalization deviations from unity are all constrained to be $\lesssim 0.2$–0.4 at 3σ CL.

If one wishes to proceed with measurements of unitarity, without the assumption of an extended U_{PMNS} matrix and its subsequent Cauchy-Schwartz constraints, then prospects for improvement are essentially limited to measuring the ν_e normalization. Improvement of all ν_e elements is possible, especially if the new generation reactor experiments, JUNO [29] and RENO50 [30], proceed as planned; see [10].

Improvements due to indirect sterile neutrino searches are promising; the Fermilab Short Baseline Neutrino [31] program, consisting of the SBND, MicroBooNE and ICARUS experiments on the Booster beam, will be capable of probing a wide range of parameter space for $3 + N$ models, increasing both the appearance and disappearance bounds. Subsequently, the long baseline program DUNE [32] will also be able to significantly extend the constrained region of $\nu_\mu \to \nu_e$ appearance to lower mass differences, leading to increased constraints on the $\nu_e\nu_\mu$ unitarity triangle in this regime. An understanding of the neutrino flux and cross-sectional uncertainties are crucial for unitarity measurements. However, no one experiment can probe all scales and complementarity is vital to definitively make a statement about unitarity from new low-energy physics. Perhaps crucially for ν_τ measurements,
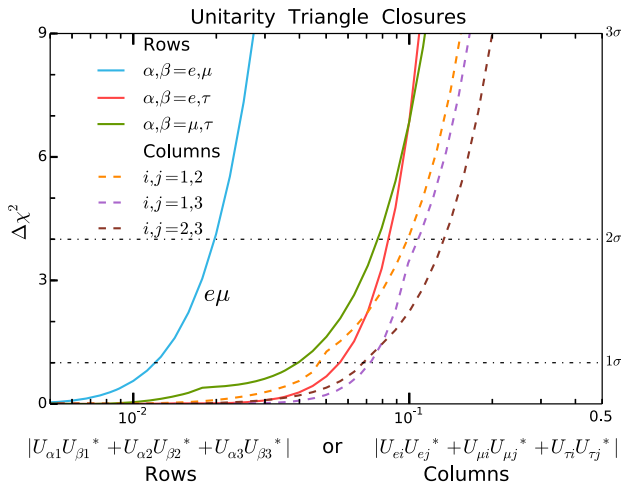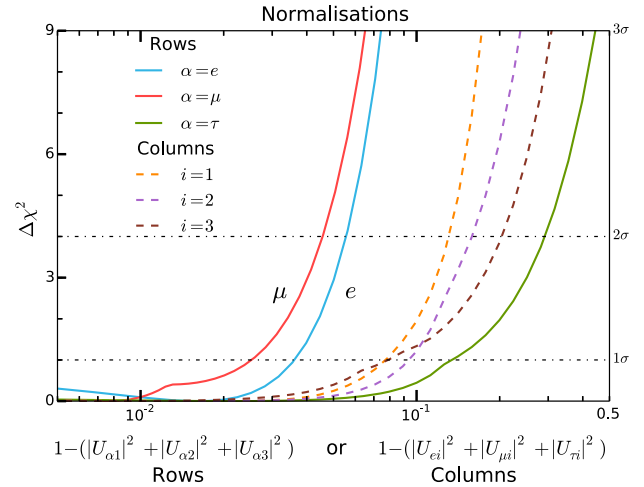

FIG. 2. 1-D $\Delta\chi^2$ for the absolute value of the closure of the three row (solid) and three column (dashed) unitarity triangles when considering new physics that enters above $|\Delta m^2| \geq 10^{-2}$ eV^2. There is one unique unitarity triangle, the $\nu_e\nu_\mu$ row unitarity triangle, in that it does not contain any ν_τ elements and hence is constrained to be unitary at a level half an order of magnitude better than the others. By comparison to Fig. 3 one can clearly see that the Cauchy-Schwartz constraints are satisfied.

Hyper-Kamiokande [33] will be quite sensitive to atmospherically averaged steriles, ≥ 0.1 eV^2, and will significantly improve the current bounds on $|U_{\tau 1}|^2 + |U_{\tau 2}|^2 + |U_{\tau 3}|^2$ in this regime, to approximately $1 - |U_{\tau 1}|^2 + |U_{\tau 2}|^2 + |U_{\tau 3}|^2 \leq 0.07$ at the 99% CL [34], which would bring all sectors in line with each other.

In this paper we have emphasized the fact that current experimental bounds on unitarity within the 3ν paradigm allow for considerable violation, and without the unitarity assumption, the precision on the individual U_{PMNS} elements can vary significantly (up to 104% in the case of $|U_{\tau 3}|$). However, we find no evidence for nonunitarity. The prospects of directly measuring all 12 unitarity constraints with high precision are poor. Currently we can only constrain the amount of nonunitarity to be $\lesssim 0.2$–0.4, for four out of six of the row and column normalizations, with the ν_μ and ν_e normalization deviations from unity constrained to be ≤ 0.07, all at the 3σ CL; see Fig. 3. Similarly, five out of six of the unitarity triangles are only constrained to be $\lesssim 0.1$–0.2, with opening of the remaining $\nu_e\nu_\mu$ unitarity triangle being constrained to be ≤ 0.03, again at

the 3σ CL; see Fig. 2. One must be careful when assessing the current experimental regime with the addition of new physics we are currently insensitive to, as without the assumption of unitarity there is much room for new effects, especially in the ν_τ sector where currently significant information comes from the unitarity assumption and not direct measurements.

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