Physical region for three-neutrino mixing angles

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We derive a set of symmetry relations for the three-neutrino mixing angles, including the Mikheyev-Smirnov-Wolfenstein (MSW) matter effect. Though interesting in their own right, these relations are used to choose the physical region of the mixing angles such that oscillations are parametrized completely and uniquely. We propose that the preferred way of setting the bounds on the mixing angles should be $\theta_{12} \in [0, \pi/2]$, $\theta_{13} \in [-\pi/2, \pi/2]$, $\theta_{23} \in [0, \pi/2]$, and $\delta \in [0, \pi)$. No CP violation then results simply from setting $\delta = 0$. In the presence of the MSW effect, this choice of bounds is a new result. Since the size of the asymmetry about $\theta_{13} = 0$ is dependent on the details of the data analysis and is a part of the results of the analysis, we argue that the negative values of θ_{13} should not be ignored.

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An abundance of data now demonstrates that neutrinos oscillate between flavor states. Analyses of the data in the context of three-neutrino mixing can be found in Refs. [1–18]. Conventionally, the standard model of the electroweak interaction is extended to include a mass term for the neutrinos and a unitary mixing matrix which relates the flavor states of the neutrinos to the mass eigenstates. We here utilize an algebraic formalism to derive symmetries of the mixing matrix which leave the predicted oscillation probabilities invariant. In particular, we are interested in understanding the bounds on the mixing angles which parametrize the mixing matrix. We derive the known bounds for the general case which includes CP violation. For the case of no CP violation, we propose a new result, for the case in which the Mikheyev-Smirnov-Wolfenstein (MSW) effect is present, of choosing the bounds as $\theta_{12} \in [0, \pi/2]$, $\theta_{13} \in [-\pi/2, \pi/2]$, $\theta_{23} \in [0, \pi/2]$, $\delta = 0$. We argue that this choice has distinct advantages for the phenomenological analysis of neutrino oscillation data.

The transformation from the mass states to the flavor states is represented by a unitary matrix $U_{\alpha j}$, $\nu_\alpha = \sum_j U_{\alpha j}\nu_j$, where we use Roman letters, j, for mass eigenstates and Greek letters, α, for flavor states. For two neutrinos, this mixing matrix reduces to an element of the commutative group $U(1)$. For vacuum oscillations, the mixing angles lie between 0 and $\pi/4$ in order to describe all discernible scenarios. For propagation in matter, this range on the mixing angle must be expanded to $[0, \pi/2]$.

In a three-neutrino theory, the mixing matrix is an element of a noncommutative group. Symmetries in the parametrization are then less obvious, especially for neutrinos propagating in matter. Transcendental expressions for locally defined mass eigenstates exist [19], but the underlying symmetries of these states are not transparent. As such, we extend the algebraic formulation of vacuum neutrino oscillations developed in [20] to include matter effects. Thus we may derive symmetries among the mixing angles and the bounds on the mixing angles which these symmetries imply. The bounds on the mixing angles are well known in vacuum; for this case, the neutrino oscillation problem is then mathematically equivalent to the quark mixing problem.

The limits on mixing angles, including the propagation through matter, have previously been considered in [21]. Our results are in agreement with theirs; however, our use of the symmetry relations permits us to arrive at additional conclusions. A discussion of the four neutrino case can be found in Ref. [22].

In [20], the vacuum oscillation probability, valid for an arbitrary fixed number of neutrino mass eigenstates, is given by

$$\mathcal{P}_{\alpha\to\beta}(t) = \frac{1}{2}\mathrm{tr}[P_+ e^{iHt} P^\alpha e^{-iHt} P_+ P^\beta], \tag{1}$$

where P^α is the flavor projection operator given by $(P^\alpha)_{jk} = (U^\dagger Q^\alpha U)_{jk} = U^*_{\alpha j} U_{\alpha k}$ in the mass-eigenstate basis, P_+ projects onto the positive-energy states, and H is an n-particle Dirac Hamiltonian for masses m_j. We note that adding multiples of the identity to the Hamiltonian leaves Eq. (1) invariant, and we recall that the trace is cyclical. For the case of three neutrinos, the relativistic limit, $p \gg m$, of the above equation is equivalent to the usual oscillation formula

$$\mathcal{P}_{\alpha\to\beta}(L/E) = \mathrm{tr}[U e^{i\mathcal{M}L/2E} U^\dagger Q^\alpha U e^{-i\mathcal{M}L/2E} U^\dagger Q^\beta] \tag{2}$$

$$\begin{aligned} &= \delta_{\alpha\beta} \\ &\quad - 4\sum_{j<k}^{3} \mathrm{Re}(U_{\alpha j}U^*_{\alpha k}U_{\beta k}U^*_{\beta j})\sin^2(\varphi_{jk}) \\ &\quad + 2\sum_{j<k}^{3} \mathrm{Im}(U_{\alpha j}U^*_{\alpha k}U_{\beta k}U^*_{\beta j})\sin(2\varphi_{jk}), \end{aligned} \tag{3}$$

where $\mathcal{M}$ is the diagonal matrix with entries (m_1^2, m_2^2, m_3^2) and $\varphi_{jk} := \Delta_{jk}L/4E$ with $\Delta_{jk} := m_j^2 - m_k^2$.

The generalization to neutrinos propagating in matter requires that the generator of time (space) translations be modified to include a flavor-dependent potential which accounts for interactions with the electrons in matter [23]. The neutral current interaction does not effect oscillations and is neglected. The charged current interaction involves only the electron flavor. As such, we must add to the Hamiltonian an effective potential which operates exclusively on the electron flavor. Explicitly, this potential is $A(x) = \sqrt{2}GE\rho(x)/m_n$, with $\rho(x)$ the electron density at position x, G the weak coupling constant, m_n the nucleon mass, and E the neutrino energy. In the mass basis, the dynamical equation in the presence of matter then becomes

$$i\partial_t \nu_m = (H + V)\nu_m = \tilde{H}\nu_m, \tag{4}$$

where V is given by $A(x)P^e$ with P^e the electron flavor projection. Given nontrivial mixing among the mass and flavor states, it is clear that the free Hamiltonian H does not commute with the potential V.

In the relativistic limit, one has $x \sim t$ so that temporal derivatives are, in effect, spatial derivatives. Formally, the solution to the differential equation in (4) is

$$\nu_m(\Gamma) = \exp\left\{-i\int_\Gamma \tilde{H} dx\right\}\nu_m(0), \tag{5}$$

where Γ parametrizes the oriented path of the neutrino through the matter with starting point $x = 0$. As the Hamiltonian is Hermitian, the adjoint of the above operator is simply $\exp\{i\int_\Gamma \tilde{H} dx\}$ which merely reverses the orientation of the path Γ.

Written in a manner akin to that in (2), the expression for the oscillation probability in matter is

$$\mathcal{P}_{\alpha\to\beta}(\Gamma, E) = \mathrm{tr}\left[\exp\left\{i\int_\Gamma U\tilde{H}U^\dagger dx\right\}Q^\alpha \exp\left\{-i\int_\Gamma U\tilde{H}U^\dagger dx\right\}Q^\beta\right]. \tag{6}$$

In the relativistic limit, the argument of the path ordered exponentials in this trace can be somewhat simplified

$$\int_\Gamma U\tilde{H}U^\dagger dx = U\mathcal{M}U^\dagger L/2E + \int_\Gamma A(x) dx Q^e, \tag{7}$$

modulo a multiple of the identity; as noted above, multiples of the identity have no physical consequence with respect to oscillations.

We use the standard parametrization of the three-neutrino mixing matrix [24]

$$U(\theta_{23}, \theta_{13}, \theta_{12}, \delta) = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix}, \tag{8}$$

where $c_{jk} = \cos\theta_{jk}$, $s_{jk} = \sin\theta_{jk}$, and θ_{jk}, δ are real. We deem equivalent two quadruples of parameters $(\theta_{23}, \theta_{13}, \theta_{12}, \delta)$ if the oscillation probabilities $\mathcal{P}_{\alpha\to\beta}(\Gamma, E)$ are identical for all values of α and β over some neutrino path Γ. This equivalence will be expressed via the relation $\equiv$. Central to our method is the fact that the trace of an operator is invariant under conjugation by any unitary U,

$$\mathrm{tr}[UAU^\dagger] = \mathrm{tr}[A]. \tag{9}$$

As the flavor projections $Q^{\alpha,\beta}$ in (6) must remain unchanged, they must commute with the conjugating matrix.

The group SO(3) has three generators. It is convenient to express the mixing matrix in terms of the exponentiated generators $U_j(\theta)$, a rotation by angle θ about the jth axis in $\mathbb{R}^3$. To account for the CP phase, we make the additional definition for $S_\delta \in \mathrm{SU}(3)$ by setting $S_\delta = \mathrm{diag}(e^{-i\delta/2}, 1, e^{i\delta/2})$ and letting

$$U_2^\delta(\theta) = S_\delta U_2(\theta) S_\delta^\dagger. \tag{10}$$

The neutrino mixing matrix (8) may be written as

$$U(\theta_{23}, \theta_{13}, \theta_{12}, \delta) = U_1(\theta_{23})U_2^\delta(\theta_{13})U_3(\theta_{12}). \tag{11}$$

From Eq. (10), we may extract our first equivalence relation. For the CP phase $\delta = \pi$, one finds

$$S_\pi U_2(\theta) S_\pi^\dagger = U_2(-\theta); \tag{12}$$

hence, one has

$$U_2^{\delta+\pi}(\theta) = U_2^\delta(-\theta). \tag{13}$$

The addition of π to the CP phase can accommodate a change in sign of θ_{13}

$$(\theta_{23}, \theta_{13}, \theta_{12}, \delta) \equiv (\theta_{23}, -\theta_{13}, \theta_{12}, \delta + \pi). \tag{14}$$

In order to proceed to further symmetries, we employ

$$U_j(\pi)U_k(\theta)U_j(\pi)^\dagger = U_k(-\theta) \tag{15}$$

for $j \neq k$; this is easily confirmed by explicit calculation. Additionally, as $U_j(\pi)$ is diagonal, it commutes with S_δ so that

$$U_j(\pi)U_2^\delta(\theta)U_j(\pi)^\dagger = U_2^\delta(-\theta) \tag{16}$$

for $j = 1, 3$.

For the same reason, $U_j(\pi)$ commutes with the mass-squared matrix $\mathcal{M}$ and the projections Q^α. The remaining step is to determine the action of $U_j(\pi)$ on the generator of spatial translations. Referring to Eq. (7), one sees that $U_j(\pi)$ commutes with the MSW potential and thus only affects the term containing the mass-squared matrix $\mathcal{M}$.

Combining these facts with Eq. (9), we see that the mixing matrices U and $U_j(\pi)^\dagger U U_j(\pi)$ yield identical oscillation probabilities. Using (15) and (16), we may express this equivalence in terms of the parameters themselves

$$(\theta_{23}, \theta_{13}, \theta_{12}, \delta) \equiv (-\theta_{23}, -\theta_{13}, \theta_{12}, \delta) \tag{17a}$$
$$\equiv (-\theta_{23}, \theta_{13}, -\theta_{12}, \delta) \tag{17b}$$
$$\equiv (\theta_{23}, -\theta_{13}, -\theta_{12}, \delta). \tag{17c}$$

From the same equations, we may determine the effect of adding π to a mixing angle. We find the following equivalence amongst parameters

$$(\theta_{23}, \theta_{13}, \theta_{12}, \delta) \equiv (\theta_{23} + \pi, \theta_{13}, \theta_{12}, \delta) \tag{18a}$$
$$\equiv (-\theta_{23}, \theta_{13} + \pi, \theta_{12}, \delta) \tag{18b}$$
$$\equiv (\theta_{23}, \theta_{13}, \theta_{12} + \pi, \delta). \tag{18c}$$

Trivially, the mixing angles satisfy a 2π periodicity; however, from the relations in (18a)–(18c), it is clear that, without loss of generality, one may further restrict all θ_{jk} to lie [25] in the interval $[0, \pi)$. In the case of θ_{13}, we are able to further narrow these bounds to $[0, \pi/2]$. An application of relation (17a) followed by (18b) yields

$$(\theta_{23}, \theta_{13}, \theta_{12}, \delta) \equiv (\theta_{23}, \pi - \theta_{13}, \theta_{12}, \delta). \tag{19}$$

In general, given a real number x, the map $x \mapsto a - x$ is a reflection about the point $a/2$ on the real line. Hence, we see that if θ_{13} should lie between $\pi/2$ and π, then the above relation shows that we have an equivalent oscillation probability for an angle reflected about $\pi/2$. In short, we may choose θ_{13} to lie in the first quadrant.

For the remaining mixing angles, we may apply relations (17b), (18a), and (18c) to achieve

$$(\theta_{23}, \theta_{13}, \theta_{12}, \delta) \equiv (\pi - \theta_{23}, \theta_{13}, \pi - \theta_{12}, \delta). \tag{20}$$

From this, one notes that a reflection about $\pi/2$ in both θ_{23} and θ_{12} results in an equivalent oscillation probability. These reflections cannot be performed independently and still result in an equivalent theory. Hence, we only have the freedom to restrict either θ_{23} or θ_{12} to the interval $[0, \pi/2]$, but not both.

Relation (20) is valid for fixed δ. Should we relax this condition on δ, then we have the liberty to restrict both mixing angles to lie between 0 and $\pi/2$. Using (14), (17a), and (18a), we have

$$(\theta_{23}, \theta_{13}, \theta_{12}, \delta) \equiv (\pi - \theta_{23}, \theta_{13}, \theta_{12}, \delta + \pi). \tag{21}$$

From similar logic, one can also deduce

$$(\theta_{23}, \theta_{13}, \theta_{12}, \delta) \equiv (\theta_{23}, \theta_{13}, \pi - \theta_{12}, \delta + \pi). \tag{22}$$

Permitting a change in the CP phase results in the ability to independently reflect these two mixing angles about $\pi/2$; hence, we are guaranteed, as noted in [21,26], that all θ_{jk} can be restricted to the interval $[0, \pi/2]$ if one allows the full range on the CP phase $\delta \in [0, 2\pi)$. This is the common understanding for the CKM mixing matrix for quarks and for neutrino oscillations including CP violation.

We propose an alternate but equivalent set of bounds for the CP violating case. As a consequence of relation (14), we see that the full range of the CP phase may be replaced by $\delta \in [0, \pi)$ by allowing a negative mixing angle $\theta_{13} \in [-\pi/2, \pi/2]$ with the two other mixing angles remaining in the first quadrant. An alternative would be to utilize Eq. (20) and allow either $\theta_{12} \in [0, \pi)$ *or* $\theta_{23} \in [0, \pi)$ with the CP phase in the first and second quadrants; however, given the smallness of θ_{13} in most models we find the extension to negative values of θ_{13} most natural.

Given that there is no indication of CP violation in neutrino oscillations, we give this case special consideration. The conventional view of taking the mixing angles $\theta_{jk} \in [0, \pi/2)$ requires that *both* $\delta = 0$ *and* $\delta = \pi$ must be included to cover the total allowed space for no CP violation, as was shown in [21]. A common oversight has been to drop the $\delta = \pi$ branch. For no CP violation it is more natural to have $\theta_{12} \in [0, \pi/2]$, $\theta_{13} \in [-\pi/2, \pi/2]$, $\theta_{23} \in [0, \pi/2]$, with only the $\delta = 0$ branch. This choice is motivated by the smallness of θ_{13}. We note that providing an upper limit on the value of $\sin^2\theta_{13}$, a common practice [24], is insufficient since $\theta_{13} < 0$ is physical and the mixing is not symmetric in θ_{13}. A two-neutrino analysis cannot distinguish the sign of θ_{13}, but a linear term in θ_{13} is present for three neutrinos and, depending on the details of the analysis, may be significant.

Experiments are not yet sensitive enough to determine the Dirac phase δ. Until there exists data to indicate a value of δ other than 0 or π in the convention of Ref. [21], or other than 0 in the convention proposed here, the special case of no CP violation is the default assumption. An example of the necessity, in principle, of incorporating the negative θ_{13} region arises from examining the question of mass hierarchy. To demonstrate this, we adopt the convention for ordering the mass eigenstates by increasing mass, $m_1 < m_2 < m_3$. This, together with the bounds chosen for the mixing angles, defines a unique basis for an analysis, i.e., each possible physical solution is included once and only once. Let us take as a typical set of parameters derived from oscillation data, $\Delta_{21} = 7 \times 10^{-5}$ eV^2, $\Delta_{32} = 3 \times 10^{-3}$ eV^2, $\theta_{12} = 0.60$, $\theta_{13} = 0.10$, and $\theta_{23} = 0.80$. This set of mass-squared differences is an example of the regular hierarchy. It is known that there is set of parameters with an inverted mass hierarchy that yield oscillation probabilities which are nearly equivalent. Using Eq. (28) in [27], we may calculate these nearly equivalent parameters $\Delta_{21} = 3 \times 10^{-3}$ eV^2, $\Delta_{32} = 7 \times 10^{-5}$ eV^2, $\theta_{12} = 1.45$, $\theta_{13} = -0.60$, and $\theta_{23} = 0.70$. We note the value of θ_{13} is negative and of relatively large magnitude. This is a consequence of choosing a fixed (ascending) mass order. Though we concede the common convention for the inverted hierarchy is to reorder the masses, the point being made here is that the resolution of the mass hierarchy question is independent of arbitrary mass ordering schemes. Utilizing a single basis, as is usually done in quantum mechanics, requires negative values of θ_{13} (or the separate branch that arises from $\delta = \pi$) to be mathematically complete and correct.

Vacuum oscillations are a special case of oscillations in matter. Consequently, they automatically satisfy the above relations. The remaining question is to determine whether there exist any additional symmetries for the vacuum case, as is in the two-neutrino theory. For three neutrinos, there are none. In our above analysis, we note that the operator $U_j(\pi)$ commutes with the MSW potential in Eq. (7). As such, the presence of this potential is inconsequential in the derivation of the symmetries that follow; hence, the special case of vanishing electron density admits no additional symmetries. To ensure that we have not overlooked a symmetry which could further reduce the bounds on the mixing angles, we have checked numerically that the mixing probabilities are indeed unique over the regions given.

In summary, we have put forth a new method for deriving symmetries of the three-neutrino mixing matrix. These symmetries are of interest themselves. They also provide an elegant way to determine the physical bounds on the mixing angles in the presence of the MSW effect. In particular, we note that a convenient way of setting these bounds is to take $\theta_{13} \in [-\pi/2, \pi/2]$, $\delta \in [0, \pi)$, and the other two angles in the first quadrant. In the case of no CP violation, where some amount of confusion appears in the literature, this reduces to setting $\delta = 0$, and taking $\theta_{13} \in [-\pi/2, \pi/2]$ with the other two angles in the first quadrant. We note that in an expansion in terms of the ratio of the small mass square difference to the large mass square difference, the lowest term is dependent only on $\sin^2\theta_{13}$. In this limit, negative θ_{13} would be redundant. However, the leading correction is linear in θ_{13}. We examine this question in Ref. [28] and find that, for reasonable parameters, the χ^2 space may have a noticeable asymmetry about $\theta_{13} = 0$, thus further motivating that the parameter space for the mixing angles be taken as derived here, a result that in the presence of the MSW effect, has not previously appeared in the literature.

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