

Unitary mixing matrices and their parameterizations

C. A. Brannen*

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Abstract

We present a new decomposition of unitary matrices particularly useful for mixing matrices. The decomposition separates the complex phase information from the mixing angle information of the matrices and leads to a new type of parameterization. We show that the mixing angle part of $U(n)$ is equivalent to $U(n - 1)$. We give closed form parameterizations for 3×3 unitary mixing matrices (such as the CKM and MNS matrices) that treat the mixing angles equally.

We show the relationship between Berry-Pancharatnam or quantum phase and the Jarlskog invariant J_{CP} that gives the CP-violation in the standard model.

We established the likely existence of the new decomposition by computer simulation in 2008. Philip Gibbs proved the $n = 3$ case in 2009 and in 2011, Samuel Lisi proved the general case using Floer theory in symplectic geometry. We give an accessible version of Lisi's proof.

* Carl.Brannen@wsu.edu

I. INTRODUCTION

We are concerned here with two problems here: (a) understanding unitary matrices from the point of view of their complex phases and information content, and (b) using this understanding to improve the parameterizations of unitary mixing matrices.

Given two bases for a finite Hilbert space, a unitary matrix defines the transformation between bases. In the case of a “mixing matrix”, the choice of bases is defined by observation. In the Standard Model of elementary particles there are two mixing matrices. The CKM mixing matrix defines how the quarks transform under the weak force, while the MNS mixing matrix does the same for the leptons. Observation of the complex phase introduced by the weak force is impossible; only the magnitude of any single matrix element can be experimentally measured.

Historically, $n \times n$ mixing matrices have been treated as a subset of the unitary matrices, $U(n)$. Parameterization of mixing matrices has been obtained by multiplying 1-parameter subgroups of $U(n)$. Such parameterizations do not form a group as they are not closed under multiplication. This paper demonstrates a more natural treatment. Rather than a *subset* of $U(n)$, here the mixing matrices form a *subgroup* isomorphic to $U(n - 1)$. As a subgroup of a Lie group, a natural parameterization is defined by exponentiation of the corresponding Lie subalgebra.

The next four sections of the paper concern unitary matrices in general: (2) the “magic” subgroup of unitary matrices $U(n)$; (3) Samuel Lisi’s proof that any unitary matrix may be put into magic form, (4) the relationship to mutually unbiased bases and Schwinger’s fictitious vacuum, and (5) the relationship between CP violation, Jarlskog invariants, and Berry-Pancharatnam phase. Sections six through eight deal with parameterizations of 3×3 unitary mixing matrices: (6) the standard parameterization; (7) the new permutation parameterization; and (8) two related parameterizations. Sections nine and ten cover applications to the CKM and MNS matrices, respectively. Section eleven is a brief conclusion.

II. MAGIC UNITARY MATRICES

For brevity, we will write the pure density matrix for the quantum state a_j as simply

$$\hat{a}_j = |a_j\rangle\langle a_j|. \tag{1}$$

We will treat the pure density matrices as the fundamental objects. Given a complete set of states $\{a_j\}$, we have equations

$$\begin{aligned}\hat{a}_j \hat{a}_k &= \delta_{jk} \hat{a}_k, \\ \sum_j \hat{a}_j &= 1,\end{aligned}\tag{2}$$

that correspond to the orthonormality and completeness relations of state vectors.

Given two complete sets of states $\{a_j\}$ and $\{b_k\}$, a unitary mixing matrix is defined by the complex numbers

$$u_{jk} = \langle a_j | b_k \rangle.\tag{3}$$

The bras and kets have arbitrary complex phases, so that under this definition, the unitary matrix will depend on these complex phases. Converting a unitary mixing matrix to a matrix of observables requires that we specify the arbitrary complex phases.

If we define a unitary matrix using pure density matrices rather than bras and kets, the arbitrary complex phases will be automatically eliminated. This will give us an observable unitary matrix.

Given a pure density matrix, we can obtain a bra or ket by taking any nonzero row or column, respectively, and normalizing. For a ket, picking a nonzero column amounts to multiplying the pure density matrix \hat{a}_j on the right by a state vector $|v\rangle$, where $|v\rangle$ has a one in a single location and all other entries zero.

It would be more convenient if we could choose $|v\rangle$ once for all the \hat{a}_j and \hat{b}_k . The requirement of “picking a nonzero column” is equivalent to requiring

$$\langle a_j | v \rangle \neq 0 \text{ and } \langle b_k | v \rangle \neq 0.\tag{4}$$

For further convenience, we require that all the above inner products have the same magnitude. For example, given $\{\langle a_j | \} = \{(1, 0), (0, 1)\}$ and $\{\langle b_k | \} = \{(\cos(\theta), \sin(\theta)), (-\sin(\theta), \cos(\theta))\}$, we could choose $\langle v | = \sqrt{1/2}(1, i)$ and have all the inner products with magnitude $\sqrt{1/2}$. In general, for a Hilbert space of dimension n , we require

$$|\langle a_j | v \rangle|^2 = |\langle b_k | v \rangle|^2 = 1/n.\tag{5}$$

In the $\{b_k\}$ basis, $|v\rangle$ is a vector whose components all have the same magnitude. So the information in the vector is in the form of the phases only.

Assuming $|v\rangle$ exists, we have that

$$\begin{aligned}\sqrt{n} \langle v | a_j \rangle &= \exp(i\alpha_j), \\ \sqrt{n} \langle b_k | v \rangle &= \exp(i\beta_k),\end{aligned}\tag{6}$$

for real angles α_j, β_k . Then the following defines the elements v_{jk} of a unitary matrix:

$$\begin{aligned} v_{jk} &= \sqrt{n} \langle v|a_j\rangle \langle a_j|b_k\rangle \sqrt{n} \langle b_k|v\rangle, \\ &= n \operatorname{tr} (\hat{v} \hat{a}_j \hat{b}_k \hat{v}). \end{aligned} \quad (7)$$

Note that $|u_{jk}|^2 = |v_{jk}|^2$ and that the two matrices are related by multiplication of rows and columns by complex phases. Since the definition uses only pure density matrices, it is free of unobservable complex phases.

Define an s -magic matrix (compare [1]) as one whose rows and columns sum to s . The unitary matrix $[v_{jk}]$ is 1-magic:

$$\sum_j v_{jk} = \sum_k v_{jk} = 1. \quad (8)$$

Multiplying an s -magic matrix by a t -magic matrix gives an st -magic matrix, so our choice of phase for the unitary matrices defines a 1-magic Lie group; we will refer to them as $MU(n)$. The corresponding Lie algebra consists of the Hermitian 0-magic matrices, $mu(n)$.

The vector of ones $x = (1, 1, \dots, 1)$, is an eigenvector of an s -magic matrix with eigenvalue s . Thus the 1-magic matrix v_{jk} transforms x to x and Eq. (7) implies that the original unitary matrix u_{jk} has a vector of phases that it transforms to another such vector. That is, for the 2-dimensional case we have:

$$\begin{pmatrix} \sqrt{2} \langle v|a_1\rangle \\ \sqrt{2} \langle v|a_2\rangle \end{pmatrix} = \begin{bmatrix} \langle a_1|b_1\rangle & \langle a_1|b_2\rangle \\ \langle a_2|b_1\rangle & \langle a_2|b_2\rangle \end{bmatrix} \begin{pmatrix} \sqrt{2} \langle b_1|v\rangle \\ \sqrt{2} \langle b_2|v\rangle \end{pmatrix}, \quad (9)$$

where $\sqrt{2} \langle b_k|v\rangle$ and $\sqrt{2} \langle v|a_j\rangle$ are the complex phases of Eq. (6). Thus the unitary matrix u_{jk} transforms the complex phases $\{\sqrt{2} \langle b_k|v\rangle\}$ to $\{\sqrt{2} \langle v|a_j\rangle\}$.

Each basis state a_j gives one real restriction on the general vector of phases:

$$|\langle v|a_j\rangle|^2 = 1. \quad (10)$$

There are n such basis state restrictions, but if the first $n - 1$ are satisfied, the last is automatic since $\sum_j \hat{a}_j = 1$. Thus we expect to find one degree of freedom left over in $|v\rangle$, which is just the vector's arbitrary complex phase. This suggests that a typical case will involve a finite number of choices for $|v\rangle$. If the bases are related, for example identical, then there may be an infinite number of choices for $|v\rangle$. In the next section we will show that such a vector of phases must exist.

There are $(n - 1)^2$ real degrees of freedom in $mu(n)$. This suggests that they are isomorphic to the Hermitian $(n - 1) \times (n - 1)$ matrices, i.e. $u(n - 1)$. To prove this, we need an Hermitian isomorphism which takes $mu(n)$ to a block diagonal form $(n - 1) \times (n - 1) + 1 \times 1$.

An Hermitian isomorphism from X to Y that preserves multiplication and addition is

$$Y = HXH^{-1} \quad (11)$$

where H is Hermitian and unitary so $H = H^{-1}$. The Householder matrices are such; they are defined as:

$$H = 1 - 2|u\rangle\langle u| \quad (12)$$

where $|u\rangle$ is a unit vector. To block diagonalize $mu(n)$ we use:

$$\begin{aligned} |u\rangle &= (u_1, u_1, \dots, u_1, u_n), \\ u_1 &= \sqrt{(\sqrt{n} + 1)/(2\sqrt{n}(n - 1))}, \\ u_n &= -\sqrt{(\sqrt{n} - 1)/(2\sqrt{n})}. \end{aligned} \quad (13)$$

Since the Householder transformation preserves multiplication and addition, it also defines an isomorphism between $MU(n)$ and $U(n - 1)$.

III. HAMILTON'S EQUATIONS

In 2008, computer calculation convinced the author that any unitary matrix can be put into magic form. The proof for $n = 2$ was trivial but higher dimensions proved recalcitrant. Philip Gibbs used geometric arguments [2] to prove the $n = 3$ case in 2009. In 2011, this author posted his conjecture, along with notes on the motivation, to an on-line mathematics website, the ‘‘Math Stack Exchange’’. Samuel Lisi soon provided a proof. [3] Lisi’s proof uses the Floer methodology of symplectic geometry. The methods used are likely to be unfamiliar (but of interest) to most working physicists so we now present a simplified version.

The proof comes in the form of a statement about the behavior of classical Hamiltonians so our first step is to translate the problem from a statement about Hilbert space into one about classical mechanics. An Hermitian matrix generates a 1-parameter subgroup of unitary matrices and any unitary matrix is an element of such a 1-parameter subgroup. Since we are translating the problem into classical mechanics we will use t for the parameter. Thus:

$$U(t) = \exp(it H_{CKM++}), \quad (14)$$

and the unitary matrix of interest is given by $U(1)$. Given an initial state $\vec{v}(0)$, the state at time t is defined by a set of coupled ordinary differential equations:

$$\vec{v}(t) = U(t)\vec{v}(0) = \exp(it H) \vec{v}(0). \quad (15)$$

The 1-parameter subgroup (and therefore the unitary matrix) are fully defined by the relationship between \vec{v} and $\dot{\vec{v}}$. In components:

$$\dot{v}_j = i \sum_k H_{jk} v_k. \quad (16)$$

Replace the complex variables with real and imaginary parts:

$$\begin{aligned} v_k &= p_k + i q_k, \\ H_{jk} &= r_{jk} + i s_{jk}. \end{aligned} \quad (17)$$

If these are compatible with a Hamiltonian \mathcal{H} , we have Hamilton's equations:

$$\begin{aligned} \dot{q}_j &= +\frac{\partial \mathcal{H}}{\partial p_j} = \sum_k (+r_{jk} p_k - s_{jk} q_k), \\ \dot{p}_j &= -\frac{\partial \mathcal{H}}{\partial q_j} = \sum_k (-r_{jk} q_k - s_{jk} p_k). \end{aligned} \quad (18)$$

Compatibility requires that $s_{jk} = -s_{kj}$ which is true since H is Hermitian. Integrating gives the Hamiltonian as:

$$\mathcal{H} = \sum_{j \neq k} (r_{jk}(p_j p_k + q_j q_k) + s_{jk} p_k q_j) + \sum_j r_{jj}(p_j^2 + q_j^2)/2. \quad (19)$$

This Hamiltonian, integrated for a period of time t , gives the unitary transformation $U(t) = \exp(iHt)$. Note that \mathcal{H} is quadratic in momentum and position and so is a generalization of an harmonic oscillator.

Mathematicians study these Hamiltonians under the label ‘‘symplectic geometry.’’ Here we give a brief and rough introduction to the mathematical language. Let $\{\hat{e}_j\}$ be a basis for the positions as a vector space. That is, given position $\vec{q} = \{q_j\}$, we treat the sum $\sum_{j=1}^n \hat{e}_j q_j$ as an element of a vector space. Similarly, let $\{\hat{f}_k\}$ be a basis for the momenta also with n elements. Combining the two basis sets gives a basis for a $2n$ -dimensional vector space M . Now define a bilinear map Ω on M which acts on the basis sets as follows:

$$\begin{aligned} \Omega(\hat{e}_j, \hat{e}_k) &= \Omega(\hat{f}_j, \hat{f}_k) = 0, \\ \Omega(\hat{e}_j, \hat{f}_k) &= -\Omega(\hat{f}_k, \hat{e}_j) = \delta_{jk}. \end{aligned} \quad (20)$$

Without Ω , M is the usual ‘‘phase space’’ of the physicists but the mathematicians prefer to call the combination a ‘‘symplectic vector space.’’

The map Ω can be thought of as a way of associating positions with momenta. That is, given two elements $u, v \in M$ with $\Omega(u, v) = 1$, we can think of u as a position and v as its associated momentum. For example, if $\Omega(q_1, p_1) = 1$, then $\Omega(p_1, q_1) = -1$ so $\Omega(p_1, -q_1) = 1$. Thus we

can think of p_1 as a position and $-q_1$ as its associated momentum. This use follows the sense of the usual canonical (or contact) transformations familiar to classical mechanics. This example is one that is typically given in textbooks on the subject; we can swap a position for its associated momentum provided we introduce a minus sign.

Classical mechanics is about the movement of systems through phase space. Suppose a system begins at some particular position. A question of interest is “can the system return to that position at time t ?” To answer this question, we consider a fixed position with all possible momenta. But Hamilton’s equations can be transformed in ways that mix position and momentum. So to understand these questions we need a definition of “initial position” that allows for any possible transformation of Hamilton’s equations.

If phase space is not transformed, then the appropriate elements of M to consider are those with the particular position and any momentum. This is easy to define by the \hat{e}_j, \hat{f}_k basis elements; we let momentum be in the subspace spanned by the \hat{f}_k . Such a subspace has dimension n , just half that of M . More generally, consider the momentum subspace resulting from any canonical transformation along with a specification of position. Such a subset of M defines an initial value problem in classical mechanics; the mathematicians call such a subset a “Lagrangian submanifold.”

We now consider the canonical transformation from q_j, p_j to ρ_j, σ_j generated by:

$$F = \left(q_j \sqrt{\rho_j^2 - q_j^2} + \rho_j^2 \sin^{-1}(q_j/\rho_j) \right) / 2. \quad (21)$$

This gives p_j and σ_j as:

$$\begin{aligned} p_j &= \frac{\partial F}{\partial q_j} = \sqrt{\rho_j^2 - q_j^2}, \\ -\sigma_j &= \frac{\partial F}{\partial \rho_j} = \rho_j \sin^{-1}(q_j/\rho_j). \end{aligned} \quad (22)$$

Solving for p_j and q_j in terms of σ_j and ρ_j we have:

$$\begin{aligned} p_j &= \rho_j \cos(\sigma_j/\rho_j), \\ q_j &= \rho_j \sin(\sigma_j/\rho_j). \end{aligned} \quad (23)$$

Putting $\rho_j = 1$ in the new coordinates defines a Lagrangian submanifold of M for which $\rho_j^2 = p_j^2 + q_j^2 = 1$. And this subset of phase space corresponds to the vectors of phases in Hilbert space. The new momentum consists of a product of n copies of complex phases so it can be called a torus; since it is also Lagrangian, it is a “Lagrangian torus”. The torus as we’ve defined it has a phase freedom. That is, if we add the same phase α to all the σ_j , the result will be a new vector that is also a vector of phases and that represents the same quantum state. This is just the usual

arbitrary complex phase present in a state vector. To eliminate it, the mathematicians prefer to identify equivalent vectors and so work with the equivalent torus in $\mathbb{C}P^{n-1}$.

Cheol-Hyun Cho[4] refers to our $\mathbb{C}P^{n-1}$ torus as a “Clifford torus”, an extension of the usual definition. His paper is perhaps the first proof that a Hamiltonian flow cannot “displace” such a torus, that is, move it in such a way that it no longer intersects with itself. Other papers that prove the existence of the intersection are [5, 6] and it can be deduced from [7–9]. This completes the proof that an unbiased state exists for two bases.

IV. MUBS AND THE FICTITIOUS VACUUM

Momentum and position are complementary observables. Perfect knowledge of one implies no knowledge of the other. Quantum information theory (QIT) studies complementary observables in the context of n -dimensional (finite) Hilbert spaces. Given two complementary bases $\{c_j\}$ and $\{d_k\}$, QIT refers to the bases as “unbiased”. Suppose we have a state c_1 . Since we can have “no knowledge” about the other observable, we must have that all the transition probabilities are equal:

$$\text{tr}(\hat{c}_1 \hat{d}_j \hat{c}_1) = \text{tr}(\hat{c}_1 \hat{d}_k \hat{c}_1). \quad (24)$$

Since $\sum_j \hat{d}_j = 1$, each of the n^2 transitions probabilities is equal to $1/n$.

A quantum state has more information than can be extracted from a single measurement. For example, spin-1/2 particles having spin in the $+x$ direction cannot be distinguished from those having spin in the $-y$ direction by using a measurement of spin in the $\pm z$ direction. However, given a large number of particles all in the same (but unknown) state, it is possible to obtain information on the state by applying different measurements to the particles. This is called “quantum tomography”. [10] For spin-1/2, the complete density matrix can be determined (approximated) by $3 = 2 + 1$ measurements; spin in the $\pm x$, $\pm y$, and $\pm z$ directions.

In terms of minimizing the number of measurements, the ideal condition for quantum tomography is to have $n + 1$ bases which are pair-wise unbiased. [11, 12] This is the maximum number of “mutually unbiased bases” (MUBs) possible, and is called a “complete set of MUBs”. Complete sets are most efficient at quantum tomography. They’ve been found for n a power of a prime but the general case is an important unsolved problem in QIT. The application of QIT to elementary particle theory is not yet even in its infancy, but see [13] for a treatment of the spin-1/2 mutually unbiased bases as an explanation for the generation structure of the masses of the quarks and

leptons. This paper continues the analysis by modernizing the treatment of the CKM and MNS matrices.

In QIT terms, we are looking for a state that is mutually unbiased with respect to the two arbitrary bases $\{a_j\}$ and $\{b_k\}$. The problem appears to be simpler than, but related to, the problem of finding complete sets of MUBs.

In the late 1950s, Julian Schwinger wrote down a version of quantum field theory that is now known as “Schwinger’s Measurement Algebra”. [14, 15] He defined a “primitive measurement” as a projection operator which cannot be written as the sum of two non zero projection operators and associated them with the elementary particles. These correspond roughly to pure density matrices. An example of a primitive measurement would be the Pauli spin projection operator for spin in the $+x$ direction, $M(+\vec{x}) = (1 + \sigma_x)/2$. In terms of a physical experiment, the primitive measurements correspond to a piece of equipment which allows particles to pass only if they possess a particular set of quantum numbers. Since the projection operators are idempotent, an incoming particle of the same type as the measurement, is left unchanged by the measurement. His theory is elegant in that it puts the states and the observables on the same mathematical footing. The related Schwinger-Weyl construction shows that three MUBs always exist in any Hilbert space of dimension larger than one. [16]

In addition to the primitive measurements $M(a_j)$, Schwinger also assumed operators where the outgoing particle is in a different state from the incoming particle $M(a_j, b_k)$. An example would be a spin raising operator $M(+\vec{z}, -\vec{z})$.

In order to provide creation and annihilation operators, Schwinger assumed the existence of a “fictitious vacuum” v . This is a state which corresponds to no particle. When the fictitious vacuum is the incoming state, we have a creation operator; when it is the outgoing state, we have an annihilation operator:

$$\begin{aligned} a_j^\dagger &= M(a_j, v) = \sqrt{n} \hat{a}_j \hat{v}, \\ a_j &= M(v, a_j) = \sqrt{n} \hat{v} \hat{a}_j. \end{aligned} \tag{25}$$

Schwinger’s work did not assume that the fictitious vacuum was in the same Hilbert space as the states. Of course it’s impossible to find a state that is unbiased with respect to all the bases of a Hilbert space. Perhaps this is why Schwinger chose the term “fictitious”.

For the case of any one particular unitary matrix, we have only two bases to consider and Schwinger’s fictitious vacuum may exist in the Hilbert space. The mathematical requirements are that all the transition probabilities are equal.

V. CP VIOLATION AND BERRY-PANCHARATNAM PHASES

Any product of pure density matrices that begins and ends with the same pure state \hat{x} is some complex number k times that pure state. We write:

$$\hat{x}\hat{y}\hat{z}\dots\hat{x} = k_{xyz\dots x} \hat{x} \quad (26)$$

where $\hat{x}, \hat{y}, \hat{z}, \dots$ are pure density matrices and $k_{xyz\dots x}$ is a number. If the left hand side happens to be zero, we define k to be zero as well. The k are observables. For example, the transition probability between \hat{x} and \hat{y} is given by $|\langle x|y\rangle|^2 = k_{yx}$.

When a quantum state is sent through a sequence of operations and then returns to its original state, it is possible for it to return multiplied by a complex phase. These are called ‘‘Berry-Pancharatnam phases’’ [17, 18] or ‘‘quantum phases’’ and are observables even though they are complex numbers. For k to have a non zero imaginary part, we must have two intermediate states.

For example, with σ_j the Pauli spin matrices, the following product of projection operators: [19]

$$\hat{z}\hat{y}\hat{x}\hat{z} = \frac{1 + \sigma_z}{2} \frac{1 + \sigma_y}{2} \frac{1 + \sigma_x}{2} \frac{1 + \sigma_z}{2}, \quad (27)$$

is a complex multiple of the projection operator $\hat{z} = (1 + \sigma_z)/2$. The observable k_{zyxz} does not depend on the choice of representation of the spin matrices; the complex constant i arises from the algebra of the Pauli spin matrices through $i = \sigma_x\sigma_y\sigma_z$. Physically, the above defines the phase $\pi/4$, picked up by a particle which navigates its way through a sequence of four Stern-Gerlach experiments oriented in the $+z$, $+x$, $+y$, and $+z$ directions.

An important example of Berry-Pancharatnam phases in elementary particles are the complex phases picked up by a fermion which emits a series of W^+ and W^- bosons. An up, charm, or top quark $\{u, c, t\}$ can emit a W^+ and become a down, strange, or bottom quark $\{d, s, b\}$:

$$\{u, c, t\} \rightarrow W^+ + \{d, s, b\}. \quad (28)$$

Similarly, the $\{d, s, b\}$ can emit a W^- :

$$\{d, s, b\} \rightarrow W^- + \{u, c, t\}. \quad (29)$$

The two types of quarks $\{d, s, b\}$ and $\{u, c, t\}$, define two bases for the 3-dimensional Hilbert space.

The transition amplitudes define a unitary matrix known as the CKM matrix:

$$V_{CKM} = \begin{pmatrix} \langle u|d\rangle & \langle u|s\rangle & \langle u|b\rangle \\ \langle c|d\rangle & \langle c|s\rangle & \langle c|b\rangle \\ \langle t|d\rangle & \langle t|s\rangle & \langle t|b\rangle \end{pmatrix} \quad (30)$$

In elementary particles literature the CKM is defined with the weak force boson interaction included so $(u, c, t)^t = V_{CKM}\gamma^0(1 - \gamma^5)/2 (d, s, b)^t$. [20] Our abbreviation is the usual QIT liberty of ignoring force bosons; either way one obtains the same V_{CKM} .

To find Berry-Pancharatnam phases in V_{CKM} we must consider transitions between pairs of states such as $\{d, s\}$ and $\{u, c\}$. For example, the observable for the transition sequence $d \rightarrow c \rightarrow s \rightarrow u \rightarrow d$:

$$\begin{aligned} k_{dusc d} \hat{d} &= \hat{d}\hat{u}\hat{s}\hat{c}\hat{d}, \text{ or} \\ k_{dusc d} &= \langle d|u\rangle\langle u|s\rangle\langle s|c\rangle\langle c|d\rangle, \\ &= V_{du} V_{su}^* V_{sc} V_{dc}^*, \end{aligned} \quad (31)$$

where V_{jk} are the entries in the CKM mixing matrix. The $k_{dusc d}$ is a Jarlskog invariant. [21] Note that $k_{dusc d}^* = k_{dcsud}$; complex conjugation reverses the ordering.

Since our states $\{u, c, t\}$ and $\{d, s, b\}$ do not include space or time dependence, the action of CP on them is reduced to the complex conjugate. Thus an observable measure of CP violation is the imaginary part of $k_{dusc d}$, which we can write as a difference between two observables:

$$J_{CP} = (k_{dusc d} - k_{dusc d}^*)/2 = (k_{dusc d} - k_{dcsud})/2. \quad (32)$$

Since $\{d, s, b\}$ form a complete basis we have:

$$\hat{s} = 1 - \hat{d} - \hat{b}. \quad (33)$$

Substituting the above in Eq. (31) and Eq. (32) we have

$$\begin{aligned} k_{dusc d} - k_{dcsud} &= (k_{du1cd} - k_{dudcd} - k_{dubcd}) - (k_{dc1ud} - k_{dcdud} - k_{dcbud}), \\ &= 0 - k_{dudcd} - k_{dubcd} - 0 + k_{dcdud} + k_{dcbud}, \\ &= k_{dcbud} - k_{dubcd}. \end{aligned} \quad (34)$$

Thus J_{CP} for transitions between $\{d, b\}$ and $\{u, c\}$ is equal to the J_{CP} for transitions between $\{d, s\}$ and $\{u, c\}$. More generally, J_{CP} is an invariant of the 3×3 CKM matrix, that is, it does not depend (except for sign) on the choice of pairs of states considered. And since we've written it in terms of pure density matrices, there is no dependence on the arbitrary complex phases of the rows and columns of the matrix. All CP violations in the quarks are proportional to J_{CP} .

VI. THE STANDARD PARAMETERIZATION FOR U(3)

After eliminating the degrees of freedom one obtains by multiplying rows and columns by complex phases, the $n \times n$ unitary matrices have $(n - 1)^2$ real degrees of freedom. Thus the 3×3 experimental unitary matrices require 4 parameters. The standard parameterization uses $\{\theta_{12}, \theta_{23}, \theta_{13}, \delta\}$:

$$\begin{aligned} c_{12} &= \cos(\theta_{12}), & c_{23} &= \cos(\theta_{23}), & c_{13} &= \cos(\theta_{13}), \\ s_{12} &= \sin(\theta_{12}), & s_{23} &= \sin(\theta_{23}), & s_{13} &= \sin(\theta_{13}), \end{aligned} \quad (35)$$

$$U_{\text{St.}} = \begin{bmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{bmatrix} \quad (36)$$

The experimentally convenient observables of the V_{CKM} consist of the transition probabilities and J_{CP} .

The $\theta_{12}, \theta_{23}, \theta_{13}$, parameters are ‘‘mixing angles’’, they correspond roughly to the probabilities that the generations change:

$$\begin{aligned} \theta_{12} &\rightarrow P_{dc}, P_{su}, \\ \theta_{23} &\rightarrow P_{st}, P_{bc}, \\ \theta_{13} &\rightarrow P_{dt}, P_{bu}. \end{aligned} \quad (37)$$

The δ parameter is intended to define CP violation. The formula for J_{CP} is:

$$J_{CP} = \sin(\delta) \sin(\theta_{23}) \sin(\theta_{13}) \sin(\theta_{12}) \cos(\theta_{23}) \cos^2(\theta_{13}) \cos(\theta_{12}). \quad (38)$$

Thus δ defines CP violation to the extent that if δ is zero, so is J_{CP} . However, setting any of the other three parameters to zero will also force $J_{CP} = 0$. Note that the above equation is almost symmetric in the mixing angles, but θ_{13} has an extra cosine factor.

VII. PERMUTATION PARAMETERIZATIONS

The usual solution to the problem of writing a subgroup of the 2×2 unitary matrices without the arbitrary complex phases is to use the real subalgebra:

$$A_\theta = \exp(i\theta \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}) = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}. \quad (39)$$

The corresponding $MU(2)$ 1-parameter subgroup is:

$$B_{2\theta} = \exp(i\theta \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}) = \frac{1}{2} \begin{bmatrix} 1 + e^{2i\theta} & 1 - e^{2i\theta} \\ 1 - e^{2i\theta} & 1 + e^{2i\theta} \end{bmatrix}. \quad (40)$$

Since A_θ and $B_{2\theta}$ have entries with the same magnitudes, they correspond to the same physical mixing matrix. We see that the real $U(2)$ matrices are a double cover of the $MU(2)$ matrices.

To convert A_θ to $B_{2\theta}$ we use two phase matrices and an overall phase $\exp(i\theta)$:

$$B_{2\theta} = e^{i\theta} \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{bmatrix} A_\theta \begin{bmatrix} 1 & 0 \\ 0 & e^{-i\pi/2} \end{bmatrix} \quad (41)$$

The Majorana phase is traditionally defined by twice the phase of the right hand phase matrix's bottom right component. In the above, that position has $\exp(-i\pi/2)$ so we see that the new Majorana phase (for 2×2 matrices) will be different from the traditional by π . Thus a calculation which obtains a Majorana phase of π such as that of Werner Rodejohann [22] (who used the full 3×3 matrices), will now obtain zero.

Since $MU(n) \equiv U(n-1)$, we can parameterize $MU(3)$ by writing down a parameterization for $U(2)$ which, in turn, can be parameterized by exponentiating its Lie algebra, $u(2)$. An arbitrary Hermitian 2×2 matrix can be parameterized as real multiples of σ_x , σ_y , σ_z and the unit matrix. Its exponential follows immediately:

$$\begin{aligned} U(2) &= \exp\left(i \begin{bmatrix} w+z & x-iy \\ x+iy & w-z \end{bmatrix}\right) \\ &= e^{iw} \begin{bmatrix} \cos(u) + iz \sin(u)/u & i(x-iy) \sin(u)/u \\ i(x+iy) \sin(u)/u & \cos(u) - iz \sin(u)/u \end{bmatrix} \end{aligned} \quad (42)$$

where $u = \sqrt{x^2 + y^2 + z^2}$.

To convert the above $U(2)$ parameterization into a Lie algebra parameterization for $MU(3)$ we use the Householder transformation of Eq. (13), to solve:

$$MU(3) = \exp\left(i \begin{bmatrix} \theta_{12} + \theta_{13} & -\theta_{12} + i\theta_{123} & -\theta_{13} - i\theta_{123} \\ -\theta_{12} - i\theta_{123} & \theta_{12} + \theta_{23} & -\theta_{23} + i\theta_{123} \\ -\theta_{13} + i\theta_{123} & -\theta_{23} - i\theta_{123} & \theta_{13} + \theta_{23} \end{bmatrix}\right) \quad (43)$$

in closed form. We obtain:

$$\begin{aligned}
MU(3) = & \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + e^{iw \frac{\cos(u)}{3}} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \\
& + e^{iw \frac{i \sin(u)}{u}} \begin{pmatrix} \phi_{23} & \phi_{12} & \phi_{13} \\ \phi_{12} & \phi_{13} & \phi_{23} \\ \phi_{13} & \phi_{23} & \phi_{12} \end{pmatrix} + e^{iw \frac{\sin(u)\theta_{123}}{u}} \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{pmatrix},
\end{aligned} \tag{44}$$

where

$$\begin{aligned}
w &= \theta_{12} + \theta_{23} + \theta_{13}, \\
\phi_{12} &= (\theta_{13} + \theta_{23} - 2\theta_{12})/3, \\
\phi_{23} &= (\theta_{12} + \theta_{13} - 2\theta_{23})/3, \\
\phi_{13} &= (\theta_{23} + \theta_{12} - 2\theta_{13})/3, \\
u &= \sqrt{3\theta_{123}^2 + 1.5(\phi_{12}^2 + \phi_{23}^2 + \phi_{13}^2)}.
\end{aligned} \tag{45}$$

A permutation matrix is a unitary matrix with all entries either zero or one. In the case of both the standard parameterization and the permutation parameterization, the three odd permutations (jk) are obtained by putting all the angles but θ_{jk} to zero. The permutation parameterization gives the even permutations (123) and (132) by arranging for all the angles but θ_{123} to be zero. Setting all the angles to zero gives the identity.

Solving for J_{CP} we find:

$$\begin{aligned}
J_{CP} = & (\phi_{12}^3 + \phi_{23}^3 + \phi_{13}^3) \cos(w) \sin^3(u)/(3u^3) \\
& + 2\theta_{123}^2 \sin(w) \cos(u) \sin^2(u)/(3u^2) \\
& + 2(\cos(w) - \cos^3(u)) \sin(w)/27,
\end{aligned} \tag{46}$$

a symmetric function of the mixing angles.

A ‘‘democratic’’ unitary matrix has all amplitudes equal in magnitude. A symmetric example is the discrete Fourier transform matrix:

$$F_3 = \sqrt{1/3} \begin{bmatrix} e^{2i\pi/3} & e^{4i\pi/3} & 1 \\ e^{4i\pi/3} & e^{8i\pi/3} & 1 \\ 1 & 1 & 1 \end{bmatrix}, \tag{47}$$

whose entries are, in general, $\sqrt{1/n} \exp(2i\pi jk/n)$. The 3×3 democratic mixing matrix happens to have the maximum possible $J_{CP} = \sqrt{3}/18$. It clearly has all mixing angles equal. The above mixing matrix is obtained (after multiplication of rows and columns by appropriate complex phases),

in the standard and the permutation parameterizations as follows:

	θ_{12}	θ_{23}	θ_{13}	δ	θ_{123}	
Standard:	$\pi/4$	$\pi/4$	0.61548	$\pi/2$.
Permutation:	$2\pi/9$	$2\pi/9$	$2\pi/9$		0	

(48)

Note that the standard parameterization must use unequal mixing angles to achieve a matrix which is the quintessential example of a mixing matrix with equal mixing angles. The permutation parameterization fixes this problem.

VIII. TWO MORE U(3) PARAMETERIZATIONS

An “ m -circulant” matrix has each row identical to the row above, but rotated m to the right. It is easily shown that any 1-magic 3×3 matrix (unitary or otherwise) can be written as the average of three magic matrices: a 1-magic matrix with all entries equal to 1, a 1-circulant 0-magic matrix defined by its top row (A_1, A_2, A_3) , and a 2-circulant 0-magic matrix with top row (B_1, B_2, B_3) :

$$\frac{1}{3} \begin{bmatrix} 1 + A_1 + B_1 & 1 + A_2 + B_2 & 1 + A_3 + B_3 \\ 1 + A_3 + B_2 & 1 + A_1 + B_3 & 1 + A_2 + B_1 \\ 1 + A_2 + B_3 & 1 + A_3 + B_1 & 1 + A_1 + B_2 \end{bmatrix}. \quad (49)$$

The above decomposition is unique and makes a natural target for a parameterization of $MU(3)$.

Let α, β, γ , and δ be four real numbers. Then:

$$\begin{aligned} A_n &= 2 \cos(\gamma) \cos((\alpha + 2n\pi)/3) e^{i\delta}, \\ B_n &= 2i \sin(\gamma) \cos((\beta + 2n\pi)/3) e^{i\delta}, \end{aligned} \quad (50)$$

gives a parameterization of $MU(3)$. The Jarlskog invariant for this parameterization is:

$$J_{CP} = (\cos(2\delta) - 2 \cos^3(\gamma) \cos(\alpha) \sin(\delta) + 2 \sin^3(\gamma) \cos(\beta) \cos(\delta))/27. \quad (51)$$

This is simpler than the permutation parameterization but does not solve the 1-parameter subgroups of $MU(3)$.

Multiplying a 1-magic unitary matrix by $e^{-i\delta}$ gives a $e^{-i\delta}$ -magic matrix. Such a transformation makes A_n pure real and B_n pure imaginary. After some algebra, this provides another parameterization of $MU(3)$:

$$U = \frac{1}{3} \begin{bmatrix} C_1 & C_2 & C_3 \\ C_3 & C_1 & C_2 \\ C_2 & C_3 & C_1 \end{bmatrix} + \frac{i}{3} \begin{bmatrix} D_1 & D_2 & D_3 \\ D_2 & D_3 & D_1 \\ D_3 & D_1 & D_2 \end{bmatrix}, \quad (52)$$

where

$$\begin{aligned} C_n &= \cos(\delta) + 2 \cos(\gamma) \cos((\alpha + 2n\pi)/3), \\ D_n &= \sin(\delta) + 2 \sin(\gamma) \cos((\beta + 2n\pi)/3). \end{aligned} \quad (53)$$

The Jarlskog invariant becomes:

$$J_{CP} = (2 \cos^3(\gamma) \sin(\delta) \cos(\alpha) + 2 \sin^3(\gamma) \cos(\delta) \cos(\beta) - \sin(2\delta))/27. \quad (54)$$

The standard parameterization is organized around the assumption that the weak force acts primarily to leave the generation number alone, and secondarily to change the generation number by 1. This is in contrast to the above, which organizes changes to the generation number as if the generations were cyclic. [13]

IX. THE CKM MATRIX

The CKM fitter group's 2009 estimates [23] for the modified Wolfenstein parameters are:

$$\begin{aligned} \lambda &= 0.2257, & A &= 0.814, \\ \bar{\rho} &= 0.135, & \bar{\eta} &= 0.349. \end{aligned} \quad (55)$$

These define the standard parameters $\{\theta_{12}, \theta_{13}, \theta_{23}, \delta\}$.

From computer calculation, we find that typical 3×3 unitary matrices can be converted to 1-magic form in four ways. Thus there are four choices for the permutation parameterization of the CKM matrix which we label according to the sign of θ_{12} and θ_{23} :

	θ_{12}	θ_{23}	θ_{13}	δ	θ_{123}
Standard	+0.22766	+0.04148	+0.00359	1.2023	
Perm ++	+0.22767	+0.04143	+0.00345		+0.00312
Perm +-	+0.22767	-0.04142	-0.00343		-0.00321
Perm -+	-0.22766	+0.04142	-0.00326		-0.00367
Perm --	-0.22766	-0.04140	+0.00320		+0.00378

(56)

The new parameters are small because the CKM matrix is near the unit matrix. In addition, the CKM matrix is very close to symmetric and this makes the θ_{123} parameter very small. Since it's not possible to distinguish the complex conjugate of the CKM matrix, there are four more choices; these have θ_{123} the same as above, while the θ_{jk} are negated. The unitary 1-magic CKM matrix is

approximately:

$$\begin{bmatrix} +0.94835 + 0.22285i & +0.05280 - 0.21946i & -0.00115 - 0.00339i \\ +0.05877 - 0.21779i & +0.93820 + 0.25917i & +0.00302 - 0.04138i \\ -0.00713 - 0.00506i & +0.00900 - 0.03971i & +0.99813 + 0.04477i \end{bmatrix}. \quad (57)$$

for the ‘‘Perm ++’’ case where all parameters are positive.

From the mixing angles Eq. (56), it’s clear that small changes to θ_{jk} for the standard parameterization correspond to equivalent small changes in the new parameterization. Near the CKM matrix, the δ angle changes approximately as:

$$\Delta\delta = 249\Delta\theta_{123} + 81\Delta\theta_{13} - 29\Delta\theta_{23} - 5.5\Delta\theta_{12}. \quad (58)$$

X. THE MNS MIXING MATRIX

In 2002, a simple form for the MNS lepton mixing matrix was proposed, the tribimaximal. [24] A tribimaximal unitary matrix has magnitudes as follows:

$$\begin{bmatrix} \sqrt{2/3} & \sqrt{1/3} & 0 \\ \sqrt{1/6} & \sqrt{1/3} & \sqrt{1/2} \\ \sqrt{1/6} & \sqrt{1/3} & \sqrt{1/2} \end{bmatrix}. \quad (59)$$

‘‘Tribimaximal’’ refers to the center and right columns, which have three and two entries, respectively, with maximal mixing. The unitary version of this matrix transforms a vector of charged lepton amplitudes $(e, \mu, \tau)^\dagger$ to a vector of neutrino amplitudes $(\nu_1, \nu_2, \nu_3)^\dagger$.

Applying the decomposition Eq. (52) to the tribimaximal amplitudes, we find a tribimaximal unitary matrix:

$$\begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & 0 \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \end{bmatrix} + i \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{-1}{\sqrt{6}} & 0 \\ \frac{-1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{3}} & \frac{-1}{\sqrt{6}} \end{bmatrix}. \quad (60)$$

This form is symmetrically divided into a real part where the values $\{1/\sqrt{3}, 1/\sqrt{6}, 0\}$ are constant over the even permutations of generation, while the imaginary part is similar, but for the odd permutations. For example, $i/\sqrt{3}$ appears in the matrix elements that correspond to the permutation (23), the swap of the 2nd and 3rd generations.

XI. CONCLUSION

Historically, unitary mixing matrices $U(n)$ have been treated as poor cousins of the unitary matrices. We've shown that they can be treated elegantly as a Lie group in their own right, equivalent to $U(n - 1)$. Rather than a parameterization scheme alone, recursion defines a new decomposition of unitary matrices into complex phases.

The traditional parameterization technique is to multiply orthogonal (real) rotations to cover as much freedom as possible, and then use complex phases to take care of what's left. In addition to being a difficult calculation (i.e. "does the parameterization cover all possible unitary matrices?"), the result is arbitrary as it depends on the multiplication order. Our new method requires only matrix exponentiation, treats all mixing angles equally, and works for all sizes of unitary matrices.

The traditional parameterization is designed to separate CP-violation from the mixing angles but in fact CP-violation depends on all the parameters. In addition, the traditional mixing angles determine the mixing correctly only in the infinitesimal limit. We show that the parameters can be chosen as defining representations of the permutation group on three elements and this makes CP-violation a secondary consequence of the mixing. Thus, in our view, theoretical attempts to derive CP-violation from a deeper theory should be focused on all the mixing angles rather than just on the 4th parameter of the traditional representation.

The CKM matrix is close to unity and this makes its parameterization less of a problem than that of the MNS matrix. For example, Bjorken, Harrison and Scott give a one parameter generalization of the tribimaximal matrix [25], Mohapatra and Yu give a two parameter generalization, [26], King gives a first-order approximation of a complete parameterization, [27] and Pakvasa, Rodejohann and Weiler give a parameterization around the tribimaximal form. [28] In this paper we provide a parameterization that has the triple advantages of treating the mixing angles equally, putting the tribimaximal matrix in a particularly symmetric form Eq. (60), and being related to a parameterization natural for the CKM matrix.

The CKM and MNS mixing matrices contribute 8 parameters; if the standard model parameters are to be derived from a deeper theory, it's important that we describe these parameters in a manner that is mathematically natural such as given in this paper. We've shown that CP-violation can be treated as a Berry-Pancharatnam or quantum phase. This defines a relationship between two important ideas, one in quantum mechanics, the other in elementary particles, and may be important for a deeper theory. We've shown that the "fictitious vacuum" of Schwinger's finite quantum field

theory “the measurement algebra” can be interpreted as the unbiased vector needed to convert a unitary matrix to magic form. In addition, an earlier paper [13] showed that picking an unbiased vector defines the arbitrary complex phases of raising and lowering operators. This suggests alternate methods of treating the vacuum of the standard model. Finally, writing the CKM matrices as a classical Hamiltonian may also be useful in a deeper theory.

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