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ON THE RECONSTRUCTION OF A UNITARY MATRIX FROM ITS MODULI:

EXISTENCE OF CONTINUOUS AMBIGUITIES

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A B S T R A C T

It is shown that, for a $n \times n$ unitary matrix with $n \geq 4$, the knowledge of the moduli of its elements is not always sufficient to determine this matrix up to "trivial" or "discrete" ambiguities. Using a parametrization "à la Kobayashi-Maskawa" in the case $n = 4$, we exhibit various configurations of the moduli for which a continuous ambiguity appears (i.e., some non-trivial phase remains free).

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The problem of reconstructing a unitary matrix U from its moduli is of obvious physical relevance. It suffices to think of U as being some scattering matrix or the quark mixing matrix appearing in the charged current of the Standard Electroweak Model [1,2]. In the latter case, though the matrix is usually taken to be 3×3 , corresponding to three generations of quarks and leptons, a larger number of generations, for instance 4, is not excluded yet by experiment.

In order to make the problem a sensible one, some trivial ambiguities have to be eliminated at once. Indeed, multiplying each row and each column of U by an arbitrary phase factor affects neither the unitarity property nor the values of the moduli. These ambiguities can be removed, for instance, by fixing the phase of each element in the first row and the first column (if U is a quark mixing matrix, such "rephasings" have no physical significance). For a $n \times n$ matrix, this means that the number of relevant free parameters has been reduced from n^2 to $n^2 - (2n-1) = (n-1)^2$. Another trivial ambiguity consists in changing U into its complex conjugate U^* .

One then observes that the number of relevant parameters coincides with the number of independent moduli (since the moduli of the last row and the last column, say, are fixed by the other ones through unitarity) [3]. Therefore, ignoring the trivial ambiguities, one can expect that the problem will have, in general, a finite number of solutions (the so-called "discrete" ambiguities). In fact, the solution is found to be unique in the (rather trivial) cases $n \leq 3$. Some partial results have been obtained when $n \geq 4$. In particular, the problem has been investigated for 4×4 matrices by using as rephasing invariant parameters the so-called "plaquette phases", first in the symmetric case $U = U^T$ [5] and recently, to some extent, in the general case [6]. When $U = U^T$ but n is arbitrary, it has been shown by Martin [7] that, if the off-diagonal moduli are not too large and not too spread out (in some precise sense), there are $2^{n(n-3)/2}$ solutions differing in a non-trivial way. Moreover, as the proof relies on the Banach-Caccioppoli principle, each solution can be constructed by iterating some contraction mapping.

The aim of this letter is to show that, for $n \geq 4$, continuous ambiguities do appear (besides the discrete ones) for certain configurations of the moduli, a point which seems to have been unnoticed so far. We also wish to emphasize that a "usual" representation of U in terms of generalized KM [2] parameters (i.e., a parametrization "à la Murnaghan" [8]) is quite suited both for the description of the non-trivial ambiguities and for actual reconstructions of U (at least when $n = 4$).

To begin with, let us produce a very simple, 4×4 example exhibiting a continuous ambiguity:

$$U = \begin{pmatrix} a & b & c & d \\ -b & a & de^{i\gamma} & -ce^{i\gamma} \\ -c & de^{i\beta} & -ae^{i(\beta+\gamma)} & be^{i\gamma} \\ -d & -ce^{i\beta} & be^{i\beta} & a \end{pmatrix} \quad (1)$$

where the real numbers a, b, c, d satisfy: $a^2 + b^2 + c^2 + d^2 = 1$. It is immediately checked that U is unitary as long as the phases β and γ are related through:

$$ac \cos \frac{\beta+\gamma}{2} = bd \cos \frac{\beta-\gamma}{2} \quad (2)$$

This means that, given the moduli $|a|$, $|b|$, $|c|$, we are left with one free, non-trivial phase (say β). Two remarks are in order. First, in (1) the matrix of the moduli is symmetric (besides other peculiarities). If one requires U itself to be symmetric, then $\beta = \gamma$ and β is determined (up to a sign) by Eq. (2): the continuous ambiguity disappears [9] [this phenomenon does not always occur, as shown by the forthcoming case B)]. Second, the set of U 's of the form (1) contains matrices for which $|b|$, $|c|$, $|d| \ll 1$: the requirement of small off-diagonal moduli does not remove the continuous ambiguity.

The previous example was (painfully!) discovered, after unsuccessful attempts to extend Martin's proof [7] to the non-symmetric case, by trying to pinpoint the origin of the disease. Afterwards, it was realized that the question of ambiguities can be discussed in a simpler and more systematic way, when $n = 4$, by using a representation "à la Murnaghan", which we now introduce. The nine relevant parameters appear as six rotation angles θ_k and three phases δ, β, γ . The explicit form is:

$$U = \begin{pmatrix} c_1 & s_1 c_3 & s_1 s_3 c_5 & s_1 s_3 s_5 \\ -s_1 c_2 & U_{22} & U_{23} & U_{24} \\ -s_1 s_2 c_4 & U_{32} & U_{33} & U_{34} \\ -s_1 s_2 s_4 & U_{42} & U_{43} & U_{44} \end{pmatrix} \quad (3a)$$

where $s_k \equiv \sin \theta_k$, $c_k \equiv \cos \theta_k$ and:

$$U_{22} = c_1 c_2 c_3 - s_2 s_3 c_6 e^{i\delta} \quad (3b)$$

$$U_{32} = c_1 s_2 c_3 c_4 + c_2 s_3 c_4 c_6 e^{i\delta} + s_3 s_4 s_6 e^{i\beta} \quad (3c)$$

$$U_{23} = c_1 c_2 s_3 c_5 + s_2 c_3 c_5 c_6 e^{i\delta} + s_2 s_5 s_6 e^{i\gamma} \quad (3d)$$

$$U_{33} = c_1 s_2 s_3 c_4 c_5 - c_2 c_3 c_4 c_5 c_6 e^{i\delta} - c_3 s_4 c_5 s_6 e^{i\beta} - c_2 c_4 s_5 s_6 e^{i\gamma} + s_4 s_5 c_6 e^{i(\beta+\gamma-\delta)} \quad (3e)$$

$$\begin{cases} U_{42} = c_1 s_2 c_3 s_4 + c_2 s_3 s_4 c_6 e^{i\delta} - s_3 c_4 s_6 e^{i\beta} \\ U_{24} = c_1 c_2 s_3 s_5 + s_2 c_3 s_5 c_6 e^{i\delta} - s_2 c_5 s_6 e^{i\gamma} \\ U_{43} = c_1 s_2 s_3 s_4 c_5 - c_2 c_3 s_4 c_5 c_6 e^{i\delta} + c_3 c_4 c_5 s_6 e^{i\beta} - c_2 s_4 s_5 s_6 e^{i\gamma} - c_4 s_5 c_6 e^{i(\beta+\gamma-\delta)} \\ U_{34} = c_1 s_2 s_3 c_4 s_5 - c_2 c_3 c_4 s_5 c_6 e^{i\delta} - c_3 s_4 s_5 s_6 e^{i\beta} + c_2 c_4 c_5 s_6 e^{i\gamma} - s_4 c_5 c_6 e^{i(\beta+\gamma-\delta)} \\ U_{44} = c_1 s_2 s_3 s_4 s_5 - c_2 c_3 s_4 s_5 c_6 e^{i\delta} + c_3 c_4 s_5 s_6 e^{i\beta} + c_2 s_4 c_5 s_6 e^{i\gamma} + c_4 c_5 c_6 e^{i(\beta+\gamma-\delta)} \end{cases} \quad (3f)$$

Equations (3) may be obtained by suitably combining six matrices of SO(4) (rotations in the six 2-planes) and two diagonal matrices of U(4). Needless to say, there are many other, similar parametrizations [10]. The one which has been chosen here is such that by setting $\theta_4 = \theta_5 = \theta_6 = 0$, U reduces to:

$$U = \left(\begin{array}{ccc|ccc} & & & 0 & & \\ & & & 0 & & \\ & & & 0 & & \\ \hline 0 & 0 & 0 & e^{i(\beta+\gamma-\delta)} & & \end{array} \right) \quad (4)$$

where the 3x3 block V is exactly the usual KM matrix.

In the expressions (3), the trivial phase ambiguities have been completely removed by setting to 0 or π the phases of the elements of the first row and the first column. In fact, one can readily convince oneself that the whole set of non-equivalent U's (modulo trivial ambiguities) is described exactly once by letting the nine parameters vary in the range: $0 < \theta_k \leq \pi/2$ ($k=1, \dots, 6$); $0 \leq \delta \leq \pi$; $-\pi < \beta, \gamma \leq \pi$. The phases δ, β, γ play here a rôle similar to that of the three independent "plaquette phases" introduced in other approaches [5,6].

The representation (3) turns out to be particularly well adapted for investigating how the matrix elements U_{ij} can be determined from the knowledge of their moduli $|U_{ij}|$. This is because the problem amounts to solve an "almost triangular" set of equations for $\theta_k, \delta, \beta, \gamma$. First of all, let us remark that the matrix elements of the last row and the last column can be completely ignored, since their seven moduli are fixed in terms of the nine other ones. This means that the information contained in Eqs. (3f) is in fact redundant for our purpose. Next,

let us assume for definiteness that none of the moduli vanishes [11], so that $s_k c_k \neq 0$ ($k=1, \dots, 5$). Then the solution can proceed through the following steps.

- (i) Starting from the upper left corner of U , we see that $|U_{11}|$, $|U_{21}|$, $|U_{12}|$, $|U_{31}|$ and $|U_{13}|$ successively fix θ_1 , θ_2 , θ_3 , θ_4 and θ_5 in a trivial and unambiguous way. Then $|U_{22}|$ determines δ as a well-defined function of θ_6 through Eq. (3b).
- (ii) Using this $\delta(\theta_6)$ in Eqs. (3c) and (3d), we find that (if no "accident" occurs) $\beta(\theta_6)$ and $\gamma(\theta_6)$ are respectively determined by $|U_{32}|$ and $|U_{23}|$ (there will be in general two solutions for β and γ).

Up to this point, the procedure is quite simple, in the sense that explicit (and not too cumbersome) expressions can be written down for δ , β , γ in terms of the still unknown parameter θ_6 (we shall not reproduce them here).

- (iii) The last step consists in inserting these expressions into Eq. (3e) and solving the resulting equation:

$$|U_{33}(\theta_6)| = \text{given value} \quad (5)$$

for θ_6 . This is the only unpleasant part of the procedure: although Eq. (5) clearly leads to an algebraic equation of the form $F(s_6) = 0$, the degree of the polynomial F is very large. Therefore, the multiplicity of the solutions θ_6 is certainly difficult to analyze on such a final form [in particular because of the spurious solutions introduced by the many squarings needed to "algebraize" Eq. (5)]. From the numerical point of view, however, there should be in principle no difficulty in solving directly the equation in the form (5).

What matters for us is rather to uncover possible continuous ambiguities. Following the previous scheme, it is obvious that the set of solutions is either finite or continuous according to whether an "accident" occurs or not in steps (ii) and (iii). In the former case, the number of solutions is bounded by the degree of F . For the reason just mentioned, we have been unable so far to study step (iii) as a potential source of continuous ambiguities. At this level, an "accident" would mean that the function $|U_{33}(\theta_6)|$ becomes θ_6 -independent for some configuration(s) of the other moduli.

As for step (ii), it is straightforward, by mere inspection of Eqs. (3c) and (3d), to analyze exhaustively how continuous ambiguities can arise there. Therefore, we shall simply state the results. Up to uninteresting changes (namely

permutations of rows or/and columns), the ambiguous configurations fall in two distinct classes:

A)

$$\delta = \pi ; \quad \vartheta_2 = \vartheta_3 , \quad \vartheta_1 = \vartheta_6 . \quad (6)$$

Then :

$$U = \begin{pmatrix} c_1 & s_1 c_2 & s_1 s_2 c_5 & -s_1 s_2 s_5 \\ -s_1 c_2 & c_1 & s_1 s_2 s_5 e^{i\gamma} & -s_1 s_2 c_5 e^{i\gamma} \\ -s_1 s_2 c_4 & s_1 s_2 s_4 e^{i\beta} & U_{33} & U_{34} \\ -s_1 s_2 s_4 & -s_1 s_2 c_4 e^{i\beta} & U_{43} & U_{44} \end{pmatrix} \quad (7)$$

where the unspecified matrix elements assume no especially simple form [they are just obtained by using (6) to eliminate δ , θ_3 and θ_6 in Eqs. (3e)-(3f)].

Equation (7) defines a 6-parameter family of unitary matrices for which there are 5 independent moduli. Four of them (say $|U_{11}|$, $|U_{21}|$, $|U_{31}|$ and $|U_{13}|$) fix θ_1 , θ_2 , θ_4 and θ_5 , one phase (say β) is free and a fifth modulus (say $|U_{33}|$) determines γ in terms of β .

One notices that the matrix of the moduli is not necessarily symmetric, although it is made of eight pairs of equal elements. Our previous example, Eq. (1), is nothing but the particular case: $\theta_4 = \theta_5$, $c_1 c_4 \cos \frac{1}{2}(\beta + \gamma) = s_1 c_2 s_4 \cos \frac{1}{2}(\beta - \gamma)$.

B)

$$\delta = 0 ; \quad \vartheta_6 = 0 , \quad c_1 = \frac{c_2 c_3}{s_2 s_3} . \quad (8)$$

Then :

$$U = \begin{pmatrix} c_1 & s_1 c_3 & s_1 s_3 c_5 & -s_1 s_3 s_5 \\ -s_1 c_2 & -s_1^2 s_2 s_3 & c_3 c_5 / s_2 & c_3 s_5 / s_2 \\ -s_1 s_2 c_4 & c_2 c_4 / s_3 & s_4 s_5 e^{i\alpha} & -s_4 c_5 e^{i\alpha} \\ -s_1 s_2 s_4 & c_2 s_4 / s_3 & -c_4 s_5 e^{i\alpha} & c_4 c_5 e^{i\alpha} \end{pmatrix} \quad (9)$$

where the angle θ_1 , still used for conciseness, is in fact that function of the parameters θ_2 , θ_3 given by Eq. (8).

Equation (9) defines a 5-parameter family of unitary matrices for which there are 4 independent moduli. The phase α [$=\beta+\gamma$ of Eq. (3)] is free.

Here, there is in general no pair of equal moduli. However, by setting $\theta_2 = \theta_3$, $\theta_4 = \theta_5$ and changing the sign of the first column in Eq. (9), we obtain a three-parameter family of symmetric matrices. In such a case, one finds that $|U_{13}|^2 + |U_{14}|^2 + |U_{23}|^2 + |U_{24}|^2 = 1$, i.e., some of the off-diagonal moduli must be relatively large in order to produce a continuous ambiguity when $U = U^T$. This is consistent with Martin's result [7], which forbids more than four (non-trivially equivalent) solutions in the symmetric case only when the off-diagonal moduli are appropriately small.

To summarize, we have exhibited, in the three-dimensional space of independent moduli, two manifolds (of dimension five and four, resp.), for which a 4×4 unitary matrix U is not determined by its moduli, even by allowing for trivial and discrete ambiguities. In particular, when the matrix of the moduli is symmetric, continuous ambiguities can occur irrespective of the magnitude of its off-diagonal elements. Of course, the set of ambiguous configuration is exceptional (of "measure zero") in the space of moduli. At the practical level, our results mean that the reconstruction of U becomes a very unstable problem when the moduli turn out to lie in the neighbourhood of the two above-mentioned manifolds. Finally, let us remind that we have no guarantee that all ambiguous configurations have been detected. In order to clear up this point within our approach, a full study of the step (iii) introduced above would be needed.

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- [10] See, e.g.: F.J. Botella and L.L. Chau - Phys.Lett. B168 (1986) 97.
- [11] When some moduli vanish, it turns out that apparent, continuous ambiguities are always removable by further rephasings.