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On the Reconstruction of a Unitary Matrix from Its Moduli

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Abstract. We study the problem of reconstructing a unitary matrix from the knowledge of the moduli of its matrix elements, first in the case of a symmetric matrix, which could be the S matrix for n coupled channels, second in the case of a non-symmetric matrix like the Cabibbo–Kobayashi–Maskawa matrix for n generations of quarks and leptons. In the symmetric case we find conditions under which the problem has $2^{(n^2-3n)/2}$ solutions differing in a non-trivial way, but also situations where one has continuous ambiguities.

In the non-symmetric case we show that for $n > 3$ there may be continuous ambiguities, of which we give an exhaustic list for $n = 4$. We give indications that there is also a set of moduli for which one has $2^{(n^2-3n)/2}$ discrete solutions, but no rigorous proof.

I. Introduction

A problem which sometimes arises in physics is that of reconstructing the phases of a unitary matrix from the knowledge of the moduli of its matrix elements. One such case is that of the S matrix for n coupled 2-body channels at a given energy and angular momentum. The problem is to find the phases of the various amplitudes when the moduli of all matrix elements, from any initial state to any final state, are known, for instance from experimental measurements. Such a problem has already been studied by one of us (G.M.) with others [1] for the case of a 4×4 matrix, where it has been discovered that the solution may be non-unique and exhibit 4-fold non-trivial ambiguities.

A related problem is that of the reconstruction of a spin zero elastic scattering amplitude from the knowledge of its modulus (i.e. the square root of the differential cross-section) at one given energy and all angles. Here one deals with an infinite matrix, but its elements are continuous, so that the problem is, in fact, simpler and, though it has not been solved completely, a lot of results have been obtained [2] and one can make the conjecture [3] that there is at most a 2-fold non-trivial ambiguity – the so-called Crichton [4] ambiguity.

In the two previous cases, one deals with unitary symmetric matrices. There is however one problem where the matrix is not necessarily symmetric, which is that of the reconstruction of the Cabibbo–Kobayashi–Maskawa matrix [5] which enters in the coupling of quarks to $W^{\pm}$ bosons, thus controlling charge current weak interactions. Naturally the K.M. matrix could be symmetric by "accident" [6]. In the 2×2 case (Cabbibo or "GIM" case [7]) the possible phases can be completely removed by a redefinition of the quark fields. In the 3×3 case, which occurs if one has 3 and only 3 generations of quarks and leptons and which is physically the most likely, both from cosmological considerations, and from the LEP experiments counting the number of light neutrinos [8], there remains one phase, after all trivial ambiguities have been removed, and this phase, once a given convention has been made on the K.M. matrix, can be obtained uniquely from the knowledge of the moduli of the K.M. matrix [9].

This is a rather remarkable fact, for it means that, by measuring moduli of decay amplitudes of all possible quarks, which is possible in principle if higher order corrections and hadronisation corrections are made, one can obtain this unique phase and, from it, one can calculate CP violating effects in K_0, Λ_0, B_0 decays. At the present time, the moduli are not sufficiently well known to lead to serious constraints on the phase, but there is no limit to the progress of experimental techniques, and the situation might change. Then one could make a consistency test between charge current decay parameters and the parameters of CP violation (ε and ε' for the $K_0 - \bar{K}_0$ system).

There remains the case of more than 3 generations of quarks and leptons, for instance 4 generations.

Though cosmology constraints forbid the existence of more than 3 species of light neutrinos and though LEP experiments exclude neutrinos with a mass inferior to $42\,\mathrm{GeV}/c^2$ [8], nothing [10] forbids the existence of a fourth family of particles with a neutrino of a mass larger than $45\,\mathrm{GeV}/c^2$. One may argue that it is not very likely. However we notice that upper limits on neutrino masses deteriorate very quickly as one goes from one family to the next, and that the top quark is certainly much heavier than expected a few years ago, with a present experimental lower limit of $90\,\mathrm{GeV}/c^2$ [11].

Anyway we do not even have to find physical excuses for studying the problem of the reconstruction of a $n \times n$ unitary matrix from the knowledge of its moduli. It is a well-defined, highly non-trivial mathematical problem, which may have different, unforeseen, physical applications.

For a unitary $n \times n$ matrix $U = \{U_{jk}\}$, we want to find out to what extent the knowledge of the moduli $|U_{jk}|$ determines U. This is the problem of *multiplicity*, to which partial answers will be given in this paper. We are not concerned here with the *consistency* problem, which amounts to obtaining necessary and sufficient conditions on the set of numbers $|U_{jk}|$ for this set to represent the moduli of a unitary matrix. Among these conditions are the trivial constraints:

$$\sum_{k=1}^{n} |U_{jk}|^2 = \sum_{k=1}^{n} |U_{kj}|^2 = 1 \quad (j = 1, \ldots, n) \tag{I.1}$$

and a set of complicated inequalities [12, 13] which will play no role here.

To begin with, one notices that there are always "trivial ambiguities," i.e. obvious changes of the phase of the U_{jk}'s which do not affect the unitarity property:

$$U \to U^*, \tag{I.2}$$

$$U_{jk} \to e^{i(\alpha_j + \beta_k)} U_{jk} \quad (\alpha_j, \beta_j \text{ arbitrary}). \tag{I.3}$$

The problem clearly makes sense only after the continuous trivial ambiguities (I.3) have been removed, e.g. by setting to zero the phases of the elements in the first row and the first column of U. In other words, any element U of the unitary group $U(n)$ can be written in a unique way as:

$$U = \begin{pmatrix} e^{i\alpha_1} & & 0 \\ & e^{i\alpha_2} \ddots & \\ 0 & & e^{i\alpha_n} \end{pmatrix} \tilde{U} \begin{pmatrix} 1 & & 0 \\ & e^{i\beta_2} \ddots & \\ 0 & & e^{i\beta_n} \end{pmatrix} \tag{I.4}$$

with $\tilde{U}_{1j} = |U_{1j}|$, $\tilde{U}_{j1} = |U_{j1}|$ $(j = 1, \ldots, n)$, and the problem amounts to determining $\tilde{U}$ from the moduli. In this way, the number of *relevant*, free (real) parameters of U is reduced from n^2 to $n^2 - (2n-1) = (n-1)^2$. But this is just the number of *independent* moduli: Eq. (I.1) contains only $(2n-1)$ independent constraints which fix, say, the moduli of the last row and the last column in terms of the other ones.

Therefore, one could expect that the problem has at most a finite number of solutions $\tilde{U}$. This is exactly what happens for $n = 2$ and 3 (it is well known that the solution is unique, up to the change (I.2) when $n = 3$). For $n \geqq 4$ however, this is not necessarily true.

In Sect. II below, it is shown that, for any n and for *symmetric* matrices ($U = U^T$), the number of solutions is finite provided that U is not too different from the unit matrix (in some precise sense). Moreover, these solutions may be obtained by iterating a contraction mapping. For $n \geqq 4$ (and general matrices U), a *continuous* set of solutions appear for certain configurations of the moduli. This means that the unitary group $U(n)$ with $n \geqq 4$ *cannot* be fully parametrized (even locally) by the set of $(n-1)^2$ independent moduli and $(2n-1)$ trivial phases (the α_j's, and β_j's of Eq. (I.4)). In the case $n = 4$, the ambiguous configurations, for which one non-trivial phase remains free, are exhaustively described in Sect. III. Some comments and further prospects are given in Sect. IV.

II. The Symmetric Case

In this section, U is assumed to be a *symmetric*, $n \times n$ matrix (with $n \geqq 4$): $U_{jk} = U_{kj}$. To avoid inessential complications, we shall also assume that *none of the moduli* $|U_{jk}|$ *vanish*. The trivial ambiguities (I.3) are then restricted to:

$$U_{jk} \to e^{i(\alpha_j + \alpha_k)} U_{jk}. \tag{II.1}$$

They can be removed e.g. by fixing the phase of the diagonal elements. This means that the number of relevant parameters is now reduced from $n(n+1)/2$ to $n(n+1)/2 - n = n(n-1)/2$, which again coincides with the number of independent moduli. More precisely we shall impose:

$$U_{jj} > 0 \; (j = 1, \ldots, n). \tag{II.2}$$

Clearly, this reduces the ambiguities (II.1) to the discrete ones,

$$U_{jk} \to e^{i\pi(n_j + n_k)} U_{jk} \quad (n_j = 0 \text{ or } 1), \tag{II.3}$$

which in turn we remove by setting:

$$U_{1k} = i|U_{1k}| e^{i\delta_{1k}} \quad \text{with} \quad -\frac{\pi}{2} < \delta_{1k} \leqq \frac{\pi}{2} \quad (k = 2, \ldots, n) \tag{II.4}$$

(such a choice is appropriate to the following treatment).

In order to investigate the reconstruction problem, it is convenient to introduce the usual "T matrix," defined by:

$$U = 1 + 2iT. \tag{II.5}$$

The unitary condition $U^+U = 1$ is then equivalent to the couple of matrix equations:

$$\frac{1}{i}(T - T^+) = T^+T + TT^+, \tag{II.6}$$

$$T^+T = TT^+. \tag{II.7}$$

The following lemma (which is true irrespective of the symmetry property $T = T^T$) will allow us to ignore condition (II.7) in our actual reconstruction procedure.

Lemma 1. *Denote by* $\|T\|$ *the operator norm of* T. *Then, if*

$$\|T\| < \frac{1}{\sqrt{2}}, \tag{II.8}$$

Eq. (*II.6*) implies Eq. (*II.7*) (*and thus the unitarity of* U).

Proof. Let us define:

$$\Delta = T^+T - TT^+ = \Delta^+.$$

Then

$$\Delta = (T^+ - T)T + T(T - T^+) = -i(T^+T^2 - T^2T^+) = -i(\Delta T + T\Delta), \tag{II.9}$$

where Eq. (II.6) has been used in the second equality.

Taking the adjoint of Eq. (II.9), we also have:

$$\Delta = i(T^+\Delta + \Delta T^+). \tag{II.10}$$

By adding Eqs. (II.9) and (II.10), and using again Eq. (II.6), we obtain:

$$2\Delta = \Delta(T^+T + TT^+) + (T^+T + TT^+)\Delta.$$

Hence, from the well-known properties of the operator norm:

$$2\|\Delta\| \leqq 2\|\Delta\|(\|T^+T\| + \|TT^+\|) \leqq 4\|\Delta\|\,\|T\|^2.$$

This means that either $\|T\| \geqq \dfrac{1}{\sqrt{2}}$ or $\Delta = 0$. q.e.d.

Remark. The bound $1/\sqrt{2}$ in Eq. (II.8) is the best possible one (in any dimension n). This is most easily seen as follows. Consider T matrices of the form:

$$T = \frac{1}{2i}\left(\begin{array}{c|c} \mathbf{a\sigma} - 1 & 0 \\ \hline 0 & 0 \end{array}\right),$$

where $\boldsymbol{\sigma}$ stands for the Pauli matrices and $\mathbf{a} = \mathbf{b} + i\mathbf{c}$ is a complex $3-$vector with $\mathbf{b}^2 + \mathbf{c}^2 = 1$. One then checks that Eq. (II.6) is always fulfilled, whereas Eq. (II.7) is true if and only if $\mathbf{b} \times \mathbf{c} = 0$. On the other hand, the norm of T is readily computed:

$$\| T \| = \frac{1}{\sqrt{2}} [1 + \sqrt{\mathbf{b}^2(1 + \mathbf{c}^2) - (\mathbf{bc})^2}]^{1/2}.$$

Clearly, $\|T\|$ can be made arbitrarily close to $1/\sqrt{2}$ by letting $|\mathbf{b}| \to 0$ (and maintaining $\mathbf{b} \times \mathbf{c} \neq 0$).

Let us now write the matrix elements of T as:

$$T_{jk} = t_{jk} e^{i\delta_{jk}} \quad (t_{jk} = t_{kj},\, \delta_{jk} = \delta_{kj}), \tag{II.11}$$

where the t_{jk}'s and the δ_{jk}'s are chosen according to the following prescriptions.

For $j = k$:

$$\delta_{jj} = \frac{\pi}{2} \quad (j = 1, \ldots, n). \tag{II.12}$$

Then $U_{jj} = 1 - 2\, t_{jj}$, so that Eqs. (I.1) and (II.2) imply:

$$0 < t_{jj} < \tfrac{1}{2}. \tag{II.13}$$

For $j \neq k$:

$$-\frac{\pi}{2} < \delta_{jk} \leqq \frac{\pi}{2}, \tag{II.14}$$

$$\begin{cases} t_{1k} > 0 & \text{(because of Eq. (II.4))} \\ t_{jk} & \textit{positive or negative } \text{for } j, k \neq 1. \end{cases} \tag{II.15}$$

Of course, the *absolute values* of the t_{jk}'s are fixed by the moduli of U:

$$\begin{cases} t_{jj} = \frac{1}{2}(1 - |U_{jj}|) \\ t_{1k} = \frac{1}{2}|U_{1k}| \\ |t_{jk}| = \frac{1}{2}|U_{jk}| \quad (2 \leqq j < k \leqq n). \end{cases} \tag{II.6}$$

The unitarity condition (II.6) reads:

$$t_{jk} \sin \delta_{jk} = \sum_{l=1}^{n} t_{jl} t_{kl} \cos(\delta_{jl} - \delta_{kl}), \quad 1 \leqq j \leqq k \leqq n. \tag{II.17}$$

Its diagonal part ($j = k$) is nothing but the set of consistency constraints (I.1), allowing us to express each t_{jj} in terms of the t_{jk}'s with $k \neq j$:

$$t_{jj} = \frac{1}{2} - \frac{1}{2}\sqrt{1 - 4 \sum_{k \neq j} t_{jk}^2}. \tag{II.18}$$

For $j \neq k$, Eq. (II.17) can be rewritten as (using Eq. (II.12)):

$$t_{jk}(1-t_{jj}-t_{kk})\sin\delta_{jk} = \sum_l{}' t_{jl}t_{kl}\cos(\delta_{jl}-\delta_{kl}), \quad 1 \leqq j < k \leqq n, \tag{II.19}$$

where $\sum_l{}'$ means that the terms with $l=j$ and $l=k$ are omitted in the sum.

This constitutes a set of $n(n-1)/2$ equations for the $n(n-1)/2$ independent unknowns δ_{jk}, ready to be solved by iteration. Actually, we are going to show that, given the t_{jk}'s:

i) Eq. (II.19) have a unique solution in the prescribed range (II.14), provided that the $|t_{jk}|$'s are properly restricted,

ii) this solution automatically fulfils the remaining unitarity condition (II.7), viz:

$$(t_{jj}-t_{kk})t_{jk}\cos\delta_{jk} = \sum_l{}' t_{jl}t_{kl}\sin(\delta_{kl}-\delta_{jl}), \quad 1 \leqq j < k \leqq n. \tag{II.20}$$

The convergence of the iterative procedure aimed at solving Eq. (II.19) can be controlled by using the contraction mapping principle. To this end, we introduce the Banach space E of $n(n-1)/2$-component vectors:

$$\delta = \{\delta_{jk}\}_{1 \leqq j < k \leqq n} \tag{II.21}$$

with the norm

$$\|\delta\| = \sup_{j,k}|\delta_{jk}|, \tag{II.22}$$

and define the mapping $\delta \to \delta' = F(\delta)$ by:

$$\sin\delta'_{jk} = \frac{1}{t_{jk}(1-t_{jj}-t_{kk})}\sum_l{}' t_{jl}t_{kl}\cos(\delta_{jl}-\delta_{kl}), |\delta'_{jk}| \leqq \frac{\pi}{2} \tag{II.23}$$

(notice that the right-hand side of these equations are well defined because of Eq. (II.13)).

Clearly, F is a mapping of E into itself as long as

$$\sum_l{}' |t_{jl}||t_{kl}| \leqq |t_{jk}|(1-t_{jj}-t_{kk}) \forall j,k \quad (j \neq k).$$

By strengthening this condition, one can enforce the mapping F to be a (strict) contraction:

Lemma 2. *Assume that*

$$\sin\mu \equiv \sup_{\substack{j,k \\ j\neq k}} \frac{\sum_l{}' |t_{jl}||t_{kl}|}{|t_{jk}|(1-t_{jj}-t_{kk})} < \frac{1}{2}. \tag{II.24}$$

Then:

i) *F maps the ball* $\|\delta\| \leqq \frac{\pi}{2}$ *into* $B \equiv \left\{\delta \,\middle|\, \|\delta\| \leqq \frac{\pi}{6}\right\}$,

ii) *F is a contraction mapping of the ball B into itself.*

Proof. i) results from trivial majorizations in Eq. (II.23).
To establish ii), consider δ, $\bar{\delta}\in B$ and $\delta' = F(\delta)$, $\bar{\delta}' = F(\bar{\delta})$.

From Eq. (II.23):

$$\sin\tfrac{1}{2}(\delta'_{jk} - \bar{\delta}'_{jk})\cos\tfrac{1}{2}(\delta'_{jk} + \bar{\delta}'_{jk}) = \tfrac{1}{2}(\sin\delta'_{jk} - \sin\bar{\delta}'_{jk})$$
$$= -\sum_l{}' \frac{t_{jk}t_{kl}}{t_{jk}(1-t_{jj}-t_{kk})}\sin\left[\tfrac{1}{2}(\delta_{jl}-\bar{\delta}_{jl}) - \tfrac{1}{2}(\delta_{kl}-\bar{\delta}_{kl})\right]$$
$$\cdot\sin\tfrac{1}{2}(\delta_{jl}+\bar{\delta}_{jl}-\delta_{kl}-\bar{\delta}_{kl}).$$

We can now use:

$$\cos\tfrac{1}{2}(\delta'_{jk}+\bar{\delta}'_{jk}) \geqq \cos\frac{\pi}{6} = \frac{\sqrt{3}}{2},$$

$$|\sin\tfrac{1}{2}(\delta_{jl}+\bar{\delta}_{jl}-\delta_{kl}-\bar{\delta}_{kl})| \leqq \sin\frac{\pi}{3} = \frac{\sqrt{3}}{2},$$

to derive:

$$\sin\tfrac{1}{2}|\delta'_{jk}-\bar{\delta}'_{jk}| \leqq \sin\mu.\sup_l \sin\tfrac{1}{2}|(\delta_{jl}-\bar{\delta}_{jl})-(\delta_{kl}-\bar{\delta}_{kl})|$$
$$\leqq \sin\mu\sin\tfrac{1}{2}\left[\sup_l|\delta_{jl}-\bar{\delta}_{jl}| + \sup_l|\delta_{kl}-\bar{\delta}_{kl}|\right]$$
$$\leqq \sin\mu\sin(\|\delta-\bar{\delta}\|).$$

Hence:

$$\sin(\|\delta'-\bar{\delta}'\|) \leqq 2\sup_{j,k}\sin\tfrac{1}{2}|\delta'_{jk}-\bar{\delta}'_{jk}| \leqq 2\sin\mu\sin(\|\delta-\bar{\delta}\|).$$

If $2\sin\mu < 1$, this entails (since $a/b \leqq \sin a/\sin b$ for $0 \leqq a \leqq b < \pi$):

$$\|\delta'-\bar{\delta}'\| \leqq 2\sin\mu\,\|\delta-\bar{\delta}\|$$

and F is a contraction. q.e.d.

We are now in a position to apply the Banach–Cacciopoli theorem and to deduce that, given a set $\{t_{jk}\}$ obeying condition (II.24), the Eqs. (II.19) have one and only one solution δ^0 in the ball $\|\delta\| \leqq \frac{\pi}{2}$ (the fixed point of F). Moreover, $\|\delta^0\| < \frac{\pi}{6}$.

It remains to show that the solution δ^0 fulfils the extra unitarity conditions, Eqs. (II.20). According to Lemma 1, this would be automatically the case, were the property (II.8) implied by condition (II.24). Such an inference however is not true. Actually, in order to derive Eq. (II.8), one would have to show that $\|t\| < \frac{1}{\sqrt{2}}$, where t is the matrix of moduli $|t_{jk}|$ (this is because the information contained in

Eq. (II.24) bears only on the moduli and because of $\|T\| \leqq \|t\|$). But counter-examples can be constructed. For instance in dimension $n=3$, the set:

$$t_{12}=t_{23}=t_{13}=\frac{1}{\sqrt{13}}, \quad t_{11}=t_{22}=t_{33}=\frac{1}{2}\left(1-\sqrt{\frac{5}{13}}\right),$$

(which obeys Eq. (II.18)) is consistent with condition (II.24) $\left(\sin\mu=\frac{1}{\sqrt{5}}\right)$, but gives

$$\|t\|=\tfrac{1}{2}[1+(4-\sqrt{5})/\sqrt{13}]>\frac{1}{\sqrt{2}}.$$

Therefore, we need some detour to establish the

Lemma 3. *Let $\{t_{jk}\}$ be a set of numbers subjected to the conditions (II.15), (II.18) and (II.24), and let $\{\delta^0_{jk}\}$ be the solution of Eqs. (II.19) in B. Then Eqs. (II.20) are satisfied by $\{\delta^0_{jk}\}$.*

Proof. For $\lambda\in(0,1]$, we define:

$$\begin{aligned} t_{jk}(\lambda) &= \lambda t_{jk} && (1\leqq j<k\leqq n),\\ t_{jj}(\lambda) &= \tfrac{1}{2}-\tfrac{1}{2}\sqrt{1-4\lambda^2 t_{jj}(1-t_{jj})} && (j=1,\dots,n) \end{aligned} \tag{II.25}$$

so that Eqs. (II.15) and (II.18) still hold for the set $\{t_{jk}(\lambda)\}$, and $t_{jk}(1)=t_{jk}\,\forall j,k$. We next denote by $\sin\mu(\lambda)$ the right-hand side of Eq. (II.24), and by F_λ the mapping defined in Eq. (II.23), $\{t_{jk}(\lambda)\}$ being substituted for $\{t_{jk}\}$ in both places. Then it is readily deduced from Eq. (II.25) that $\sin\mu(\lambda)$ is an increasing function of λ. Hence:

$$\sin\mu(\lambda)<\sin\mu(1)=\sin\mu<\tfrac{1}{2}.$$

Therefore, according to Lemma 2, F_λ is a contraction mapping $B\to B$ and the equation $\delta=F_\lambda(\delta)$ has a unique solution $\delta(\lambda)\in B$, with $\delta(1)=\delta^0$.

Now, Eqs. (II.23) and (II.25) show that the function $(0,1]\times B\to B$ defined by $F_\lambda(\delta)$ is analytic both in λ and δ. Moreover, the derivative of $1-F_\lambda$ is invertible at any point $\lambda\in(0,1]$ (otherwise F_λ would not be a contraction there). The "holomorphic" implicit function theorem then tells us that $\delta(\lambda)$ itself is analytic on $(0,1]$.

On the other hand, we have from Eq. (II.25):

$$t_{jk}(\lambda)\underset{\lambda\to 0}{=}O(\lambda), \quad 1\leqq j\leqq k\leqq n,$$

so that $\|T(\lambda)\|<\frac{1}{\sqrt{2}}$ for λ small enough. According to Lemma 1, this means that Eqs. (II.20) (written for $\{t_{jk}(\lambda)\}$ and $\delta(\lambda)$) are satisfied when λ is small enough. Since both sides of Eq. (II.20) are analytic functions of λ, these equations are identically true for all $\lambda\in(0,1]$, in particular for $\lambda=1$. q.e.d.

Knowing that a given set $\{t_{jk}\}$ (obeying the condition (II.24)) produces a unique solution δ^0 and provides us with a unitary matrix U, we can now come back to our initial problem and count the number of its solutions for a given set of moduli $|U_{jk}|$. Let us recall that the signs of certain off-diagonal elements t_{jk} are still arbitrary:

$$t_{jk} = \pm \tfrac{1}{2}|U_{jk}| \quad \text{for} \quad 2 \leqq j < k \leqq n.$$

Choosing these signs in all possible ways, we obtain $2^{(n-1)(n-2)/2}$ different solutions δ. These solutions however are pairwise related by a trivial change of phases. Actually, one observes that Eqs. (II.19) are invariant under the substitution.

$$\begin{cases} t_{jk} \to -t_{jk} & 2 \leqq j < k \leqq n \\ \delta_{jk} \to -\delta_{jk} & 1 \leqq j < k \leqq n \end{cases}$$

and that this substitution is nothing but a trivial change combining (I.2) and (II.1) and respecting our prescriptions (II.2) and (II.4):

$$U_{jk} \to (-1)^{\delta_1^j + \delta_1^k} U^*_{jk} \quad \text{(here, } \delta_1^j \text{ stands for the Kronecker symbol).}$$

Consequently, the sign of a further t_{jk} can be fixed (e.g. $t_{23} > 0$), and there are only $\frac{1}{2}2^{(n-1)(n-2)/2} = 2^{n(n-3)/2}$ solutions differing in a non-trivial way.

Collecting our results, we can assert:

Theorem 1. *Let the moduli $|U_{jk}|$ of a symmetric, $n \times n$ matrix ($n \geqq 4$) be given. Assume that Eqs. (I.1) hold and that:*

$$\sum_{\substack{l=1,\ldots,n \\ l \neq j,k}} |U_{jl}||U_{kl}| < \tfrac{1}{2}|U_{jk}|(|U_{jj}| + |U_{kk}|), \quad 1 \leqq j < k \leqq n. \tag{II.26}$$

Then, up to trivial ambiguities (I.2) and (II.1), there are $2^{n(n-3)/2}$ unitary matrices U having these $|U_{jk}|$'s as moduli. These matrices can be constructed as follows.

Define:

$$\begin{aligned} t_{jj} &= \tfrac{1}{2}(1 - |U_{jj}|) & j &= 1 \ldots n, \\ t_{1k} &= \tfrac{1}{2}|U_{1k}| & k &= 2 \ldots n; & t_{23} &= \tfrac{1}{2}|U_{23}|, \\ t_{jk} &= \tfrac{1}{2}\varepsilon_{jk}|U_{jk}| & j &= 2, 4 \leqq k \leqq n; & 3 &\leqq j < k \leqq n, \end{aligned} \tag{II.27}$$

and choose $\varepsilon_{jk} = \pm 1$ in all possible ways. For each choice, solve iteratively Eqs. (II.19), starting from any set $\{\delta_{jk}^{(1)}\}$ with $|\delta_{jk}^{(1)}| \leqq \frac{\pi}{6}$. The iteration sequence $\{\delta_{jk}^{(p)}\}$ converges to a unique solution $\{\delta_{jk}\}$ $\left(\text{with} |\delta_{jk}| < \frac{\pi}{6}\right)$.

Then:

$$\begin{cases} U_{jj} = |U_{jj}|, & j = 1, \ldots, n, \\ U_{1k} = i|U_{1k}|e^{i\delta_{1k}}, & k = 2, \ldots, n, \\ U_{23} = i|U_{23}|e^{i\delta_{23}}, & \\ U_{jk} = 2it_{jk}e^{i\delta_{jk}} & \textit{for the remaining indices.} \end{cases} \tag{II.28}$$

Finally, let us make more explicit the rough meaning of condition (II.26): the off-diagonal moduli $|U_{jk}|$ are required to be both not too large and not too different from each other.

III. The Continuous Ambiguities for 4 × 4 Matrices

So far, the reconstruction problem in the general (non-symmetric) case has resisted all attempts to generalize the approach of the previous section. A reason for the difficulty was discovered in Ref. [14]: when $n \geqq 4$, a continuous set of solutions appears for certain configurations of the moduli. Some of these ambiguous configurations were displayed. We have now completed this work by searching for all ambiguous configurations in the case $n = 4$, and we can report on the outcome. Unfortunately, we were unable to set up a simple method for dealing with this problem, which was solved by brute force calculations. There is no point in reproducing here these long computations, and we shall merely summarize the main steps.

We have found it convenient to follow two routes simultaneously. The first one is based on a generalized Kobayashi–Maskawa (KM) parametrization of 4 × 4 unitary matrices U [15]. In the second one, we use the unitarity equations in the form given by Lavoura [16]. Let us describe successively these two approaches.

In the KM representation, the 9 relevant parameters of U are 6 rotation angles θ_k and 3 phases δ, β, γ.

The explicit form we have chosen is:

$$U = \begin{pmatrix} c_1 & s_1 c_3 & s_1 s_3 c_5 & s_1 s_3 s_5 \\ -s_1 c_2 & U_{22} & U_{23} & U_{24} \\ -s_1 s_2 c_4 & U_{32} & U_{33} & U_{34} \\ -s_1 s_2 s_4 & U_{42} & U_{43} & U_{44} \end{pmatrix} \tag{III.1a}$$

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

$$U_{22} = c_1 c_2 c_3 - s_2 s_3 c_6 e^{i\delta}, \tag{III.1b}$$

$$U_{32} = c_1 s_2 c_3 c_4 + c_2 s_3 c_4 c_6 e^{i\delta} + s_3 s_4 s_6 e^{i\beta}, \tag{III.1c}$$

$$U_{23} = c_1 c_2 s_3 c_5 + s_2 c_3 c_5 c_6 e^{i\delta} + s_2 s_5 s_6 e^{i\gamma}, \tag{III.1d}$$

$$U_{33} = c_1 s_2 s_3 c_4 c_5 - c_2 c_3 c_4 c_5 c_6 e^{i\delta} - c_3 s_4 c_5 s_6 e^{i\beta} - c_2 c_4 s_5 s_6 e^{i\gamma} + s_4 s_5 c_6 e^{i(\beta+\gamma-\delta)}, \tag{III.1e}$$

$$\begin{aligned}
U_{42} &= c_1 s_2 c_3 s_4 + c_2 s_3 s_4 c_6 e^{i\delta} - s_3 c_4 s_6 e^{i\beta}, \\
U_{24} &= c_1 c_2 s_3 s_5 + s_2 c_3 s_5 c_6 e^{i\delta} - s_2 c_5 s_6 e^{i\gamma}, \\
U_{43} &= c_1 s_2 s_3 s_4 c_5 - c_2 c_3 s_4 c_5 c_6 e^{i\delta} + c_3 c_4 c_5 s_6 e^{i\beta} - c_2 s_4 s_5 s_6 e^{i\gamma} - c_4 s_5 c_6 e^{i(\beta+\gamma-\delta)}, \\
U_{34} &= c_1 s_2 s_3 c_4 s_5 - c_2 c_3 c_4 s_5 c_6 e^{i\delta} - c_3 s_4 s_5 s_6 e^{i\beta} + c_2 c_4 c_5 s_6 e^{i\gamma} - s_4 c_5 c_6 e^{i(\beta+\gamma-\delta)}, \\
U_{44} &= c_1 s_2 s_3 s_4 s_5 - c_2 c_3 s_4 s_5 c_6 e^{i\delta} + c_3 c_4 s_5 s_6 e^{i\beta} + c_2 s_4 c_5 s_6 e^{i\gamma} + c_4 c_5 c_6 e^{i(\beta+\gamma-\delta)}.
\end{aligned} \tag{III.1f}$$

In Eqs. (III.1), the trivial ambiguities (I.3) have been removed by setting to 0 the phases of $U_{1k} (k = 1, \ldots, 4)$ and to π the phases of $U_{j1} (j = 2, 3, 4)$. In fact, a whole set of non-equivalent U's (modulo the changes (I.2) and (I.3)) is described exactly once by letting the parameters vary in the range:

$$\begin{cases} 0 \leqq \theta_k \leqq \dfrac{\pi}{2} \quad (k = 1 \ldots 6) \\ 0 \leqq \delta \leqq \pi; \quad -\pi < \beta, \quad \gamma \leqq \pi \end{cases} \tag{III.2}$$

(notice that these phase fixing conventions differ from those of Eq. (I.4); the parametrization chosen here is merely an extension of the usual KM representation [5], which appears in the upper left 3×3 block of (III. 1a) when $\theta_4 = \theta_5 = \theta_6 = 0$).

Given the set of moduli $|U_{jk}|$, we can now try to solve for the parameters θ_k, δ, β, γ. Again, we shall assume that $|U_{jk}| \neq 0 \, \forall j, k$, i.e. $s_k c_k \neq 0$ for $k = 1, \ldots, 5$ (when some moduli vanish, one finds that apparent, continuous ambiguities are always removable by further rephasings). The representation (I.1) turns out to be well adapted to our purpose, because the equations to solve form an almost triangular set. First of all, we are allowed to ignore the matrix elements of the last row and the last column, since their seven moduli are fixed by the nine other ones through Eq. (I.1) (this means that the information contained in Eqs. (III.1f) is in fact redundant for the reconstruction problem). Then the solution can proceed through the following steps.

S1) 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 an unambiguous way. Then $|U_{22}|$ determines δ as a well-defined function of c_6 as long as $\theta_6 \neq \dfrac{\pi}{2}$:

$$\cos\delta = \frac{(c_1 c_2 c_3)^2 + (s_2 s_3 c_6)^2 - |U_{22}|^2}{2 c_1 s_2 c_2 s_3 c_3 c_6} \tag{III.3}$$

$\left(\text{if } \theta_6 = \dfrac{\pi}{2}\right.$, the phase δ simply disappears from U, whereas β and γ are univocally fixed by $|U_{32}|$ and $\left.|U_{23}|\right)$.

S2) Using the expression (III.3) in Eqs. (III.1c) and (III.1d), we find that, *if no "accident" occurs*, β and γ are respectively determined by $|U_{32}|$ and $|U_{23}|$ as algebraic functions of the still unknown parameter c_6:

$$\begin{aligned} \cos\beta &= f(c_6), \\ \cos\gamma &= g(c_6). \end{aligned} \tag{III.4}$$

Up to this point, the procedure is simple, in the sense that the explicit forms of f and g are not exceedingly heavy (in fact, each of these functions is double-valued, because of square-rootings).

S_3) In the last step, one has to insert the expressions (III.3) and (III.4) into the right-hand side of Eq. (III.1e), which provides us with a function $h(c_6)$, and to solve:

$$|h(c_6)|^2 = |U_{33}|^2 \tag{III.5}$$

for c_6.

This is the unpleasant part of the procedure: although the algebraic equation

(III.5) can clearly be put in the form:

$$F(c_6) = 0, \tag{III.6}$$

where F is a polynomial, the coefficients of F are very cumbersome (polynomial) functions of the moduli. The degree of F is *twelve*, and it can be shown that the squarings needed to go from Eq. (III.5) to Eq. (III.6) introduce no spurious solutions: they just account for the double valuedness appearing in step S_2. This means that Eqs. (III.3), (III.4) and (III.6) exactly solve our initial problem. Again, if no "accident" occurs, Eq. (III.6) will fix the value(s) of δ_6.

Let us be more explicit about what is meant by "accidents." In step S_2, it may happen that β and/or γ are not fixed by $|U_{32}|$ and $|U_{23}|$ (the functions f and/or g do not exist). For instance, if it turns out that $\delta = \pi$ and $c_6 = c_1 s_2 c_3 / c_2 s_3$, we see from Eq. (III.1c) that β remains free at this level. Then, one has to proceed further in order to establish whether β and γ are fixed by the other equations or not. In the latter case, we shall say that an accident has occurred in step S_2.

As for step S_3, the occurrence of an accident there simply means that Eq. (III.6) reduces to an identity (all the coefficients of the polynomial F vanish), keeping c_6 undetermined.

Clearly, we are left with the following alternative:

i) No accidents are encountered in steps S_2 and S_3. Then *there are at most* 12 *solutions.*

ii) An accident occurs in step S_2 or in step S_3. Then *the set of solutions is continuous.*

The case i) corresponds to the "discrete ambiguities," which have been investigated by Lavoura [17]. There it was shown that the number of solutions is even (in the generic case). No upper bound on this number was derived, but the configurations of the moduli studied numerically never produced more than 8 solutions, including complex conjugations.

Let us turn to case ii). By mere inspection of Eqs. (III.1c–e), it is straightforward to analyse exhaustively how an accident can occur in step S_2. The resulting ambiguous configurations belong to the classes denoted by A) and B) in Theorem 2 below.

The task of analysing step S_3 is much more difficult, and it is at this point that we appeal to the second approach. Actually, instead of looking at the explicit form of Eqs. (III.5–6), we have found it a little more convenient to utilize the set of unitarity equations given in ref. [16], which involve more directly the moduli.

For the sake of conciseness, the matrix of *squared* moduli is denoted by:

$$\{|U_{jk}|^2\} = \begin{pmatrix} A & B & C & D \\ E & F & G & H \\ I & J & K & L \\ M & N & O & Q \end{pmatrix} \tag{III.7}$$

and the 9 independent elements are chosen again in the upper left 3×3 block. The basic parameters to be determined by unitarity are:

$$\begin{cases} \varphi = (\delta_{11} - \delta_{12}) - (\delta_{21} - \delta_{22}), \\ \omega = (\delta_{11} - \delta_{13}) - (\delta_{21} - \delta_{23}), \\ \chi = (\delta_{11} - \delta_{12}) - (\delta_{31} - \delta_{32}). \end{cases} \tag{III.8}$$

These 3 "plaquette phases" (which are invariant against rephasings (I.3)) play the same role as our KM phases δ, β, γ. In ref. [16], it was shown that the unitarity of U is equivalent to the set of trigonometric equations:

$$\begin{cases} b_1 \cos\varphi + b_2 \cos\omega + b_3 \cos(\omega - \varphi) = d_1, \\ c_1 \cos\varphi + c_2 \cos\chi + c_3 \cos(\chi - \varphi) = d_2, \\ a_1 \cos\varphi + a_2 \cos\omega + a_1 \cos\chi + a_4 \cos(\omega - \chi) + a_5 \cos(\varphi - \omega - \chi) = d_3, \end{cases} \tag{III.9}$$

provided that the subdeterminant $U_{13}U_{24} - U_{14}U_{23}$ does not vanish. Moreover, once a solution of these equations has been obtained with $0 \leqq \varphi \leqq \pi$, $-\pi < \omega, \chi \leqq \pi$, U is univocally fixed (up to the trivial changes (I.2) and (I.3)). In Eq. (III.9), the expressions of the coefficients in terms of the independent moduli are[1]:

$$\begin{cases} b_1 = 2\sqrt{ABEF}, \quad b_2 = 2\sqrt{ACEG}, \quad b_3 = 2\sqrt{BCFG}, \\ d_1 = 1 - A - B - C - E - F - G + AF + AG + BE + BG + CE + CF, \\ c_1 = b_1, \quad c_2 = 2\sqrt{ABIJ}, \quad c_3 = 2\sqrt{EFIJ}, \\ d_2 = 1 - A - B - E - F - I - J + AF + AJ + BE + BI + EJ + FI, \\ a_1 = (1 - C - I - K)b_1, \quad a_2 = (J - I)b_2, \quad a_3 = (G - C)c_2, \\ a_4 = -2\sqrt{BCEGIJ}, \quad a_5 = -2\sqrt{ACFGIJ}, \\ d_3 = 1 - A - B - C - E - F - I - K + AF + BE + CI - GJ \\ \qquad + AGJ - AGI - ACJ - BCI - CEI - CFI \\ \qquad + (C + I + K)(A + B + E + F - AF - BE). \end{cases} \tag{III.10}$$

Now, following the previous approach, it is readily seen that if some subdeterminant of order 2 vanishes in U, the only ambiguous configurations fall in the class B) below. Therefore, with the purpose of uncovering all possible ambiguities hidden in step S_3, we can safely stick to Eqs. (III.9). Eliminating ω and χ between them, one obtains for the remaining variable $x = \cos\varphi$ an equation of the form:

$$\prod_{\substack{\varepsilon = \pm 1 \\ \nu = \pm 1}} [Q_3(x) + \varepsilon T_1(x)\sqrt{(1 - x^2)R_2(x)} + \nu U_1(x)\sqrt{(1 - x^2)r_2(x)} \\ + \varepsilon\nu S_1(x)\sqrt{R_2(x) r_2(x)}] = 0, \tag{III.11}$$

where $Q_3(x)$, $T_1(x)$, $R_2(x)$,... are polynomials, the degree of which is indicated by the indices 3, 1, 2,... (and the coefficients of which are themselves polynomial functions of the moduli). This equation is very similar (and completely equivalent) to the explicit form of Eq. (III.6), but it is slightly more compact when fully detailed. Through expansion of the products, it appears as a 12^{th} degree algebraic equation. The best strategy however consists of using the factorized form (III.11). A new continuous ambiguity (x free) will occur each time the moduli can be so adjusted that one of the four factors identically vanishes. This may happen in various ways, e.g. by identical vanishing of all four polynomials Q_3, T_1, U_1 and S_1, or through proportionality relations between $(1 - x^2)$, $R_2(x)$ and $r_2(x)$. All these possibilities must be systematically explored, which is extremely long because there are many

[1] Equations (III.9–10) are the "master equations" of Lavoura, rewritten here in a slightly different way

ramifying cases and cumbersome functions of the moduli to deal with. Of course, such an extensive calculation cannot be reproduced here, and we shall content ourselves with quoting the (simple!) result: besides ambiguous configurations falling again in classes A) and B), only one new type is discovered, namely the class C) displayed below.

Our whole analysis can be summed up by the following theorem.

Theorem 2. *Let the moduli of a unitary* 4×4 *matrix be given*:

$$\{|U_{jk}|\} = \begin{pmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ m & n & p & q \end{pmatrix} \tag{III.12}$$

(*the* 9 *moduli in the upper left* 3×3 *block can be taken as the independent ones*). *Then, up to trivial ambiguities* (*I*.2) *and* (*I*.3), *there are either*

i) *at most twelve unitary matrices* U

or

ii) *a continuous set of unitary matrices* U
having these $|U_{ik}|$'*s as moduli.*

The case ii) is encountered if and only if U belongs to one of three classes A), B) and C). Each class is obtained from the matrices described below (within the parametrization (III.1)) by arbitrary permutations of rows, permutations of columns and transpositions.

For A):

$\delta = \pi$, $\theta_2 = \theta_3$, $\theta_1 = \theta_6$; that is:

$$U = \begin{pmatrix} c_1 & s_1 c_2 & s_1 s_2 c_5 & s_1 s_2 s_5 \\ -s_1 c_2 & c_1 & s_1 s_2 s_5 \, e^{i\gamma} & -s_1 s_2 c_5 \, e^{i\gamma} \\ -s_1 s_2 c_4 & s_1 s_2 s_4 \, e^{i\beta} & U_{33} & U_{34} \\ -s_1 s_2 s_4 & -s_1 s_2 c_4 \, e^{i\beta} & U_{43} & U_{44} \end{pmatrix}, \tag{III.13}$$

where the unspecified elements assume no particularly simple forms (they are just obtained by using (III.13) in Eqs. (III.1e – f)). *One phase* (say β) is *free* and $|U_{33}|$ determines γ in terms of β.

The configuration of moduli exhibits the "symmetric" pattern:

$$\{|U_{jk}|\} = \begin{pmatrix} a & b & c & d \\ b & a & d & c \\ i & j & k & l \\ j & i & l & k \end{pmatrix} \tag{III.14}$$

Five of them are *independent* (say, a, b, c, i and k).

For B):

$\delta = 0$, $\theta_6 = 0$, $c_1 = \dfrac{c_2 c_3}{s_2 s_3}$; that is:

$$U=\begin{pmatrix} c_1 & s_1 c_3 & s_1 s_3 c_5 & s_1 s_3 s_5 \\ -s_1 c_2 & -s_1^2 s_2 s_3 & c_3 c_5/s_2 & c_3 s_5/s_2 \\ -s_1 s_2 c_4 & c_2 c_4/s_3 & s_4 s_5\, e^{i\alpha} & -s_4 c_5\, e^{i\alpha} \\ -s_1 s_2 s_4 & c_2 s_4/s_3 & -c_4 s_5\, e^{i\alpha} & c_4 c_5\, e^{i\alpha} \end{pmatrix}, \tag{III.15}$$

where θ_1 is still used for conciseness.

The phase $\alpha(=\beta+\gamma)$ *is free.*

There are in general no pairs of equal moduli. However, they are constrained by 5 relations:

$$af=be,\ ch=dg,\ in=jm,\ kq=lp,$$
$$a^2+b^2+e^2+f^2=1, \tag{III.16}$$

so that *four* of them remain *independent.*

For C):

$$c_3=\frac{c_1}{s_1},\quad \theta_5=\frac{\pi}{4}, \tag{III.17}$$

δ, β and γ are expressed in terms of the *variable* parameter θ_6 through:

$$\begin{cases} \cos\delta=\dfrac{s_3(s_2^2c_6^2-c_2^2)}{2c_1c_2s_2c_3c_6}, \\ \cos(\beta-\nu)=\dfrac{s_3(c_4^2-s_4^2)s_6}{2c_4s_4\sqrt{s_1^2s_2^2-s_3^2s_6^2}} \quad \text{where} \quad \cos\nu=\dfrac{2s_1^2s_2^2-s_2^2s_3^2s_6^2}{2c_1s_2c_3\sqrt{s_1^2s_2^2-s_3^2s_6^2}} \\ tg\gamma=-s_1s_3\sqrt{\dfrac{s_2^2c_6^2-s_1^2c_2^2s_3^2}{c_2^2-s_1^2s_2^2s_3^2c_6^2}}, \quad \text{and} \quad 0\leqq\nu\leqq\pi, \end{cases} \tag{III.18}$$

so that *one phase* remains free.

The configuration of moduli is characterized by two pairs of identical columns:

$$\{|U_{jk}|\}=\begin{pmatrix} a & a & \sqrt{\frac{1}{2}-a^2} & \sqrt{\frac{1}{2}-a^2} \\ e & e & \sqrt{\frac{1}{2}-e^2} & \sqrt{\frac{1}{2}-e^2} \\ i & i & \sqrt{\frac{1}{2}-i^2} & \sqrt{\frac{1}{2}-i^2} \\ m & m & \sqrt{\frac{1}{2}-m^2} & \sqrt{\frac{1}{2}-m^2} \end{pmatrix}. \tag{III.19}$$

The *three* moduli a, e, i, are *independent.*

Let us summarize the main result of this section. We have found all the cases in which a unitary 4×4 matrix is not determined by its moduli, even by allowing for trivial or discrete ambiguities. Taking into account the possible rearrangements and the various "symmetries" of the matrices corresponding to Eqs. (III.14), (III.16) and (III.19), we see that the set of ambiguous configurations is made of 24 manifolds in the 9 dimensional space of independent moduli. There are 9 manifolds of dimension 5 (class A)), 9 of dimension 4 (class B)) and 6 of dimension 3 (class C)). Although these ambiguous configurations are exceptional (of "measure zero"), it is important to realize that the reconstruction of U becomes a very unstable problem when the moduli turn out to lie in the vicinity of the above-mentioned manifolds.

It is also worth stressing the following points:

1. For non-symmetric matrices U, requiring that the off-diagonal moduli be small enough does not prevent the occurrence of continuous ambiguities. Counter-examples are immediately found in class A), since b, c, d and can be chosen arbitrarily small in the matrix (III.14).

2. Obviously, Theorem 2 still applies in the symmetric case $U = U^T$: it suffices (after changing the sign of the first column in (III.1a) to set everywhere $\theta_2 = \theta_3$, $\theta_4 = \theta_5$, $\beta = \gamma$. If we take for instance, case (C), the symmetric matrix

$$\begin{pmatrix} a & ae^{i\phi_1} & be^{i\phi_2} & be^{i\phi_3} \\ ae^{i\phi_1} & a & be^{i\phi_3} & be^{i\phi_2} \\ be^{i\phi_2} & be^{i\phi_3} & a & ae^{i\phi_1} \\ be^{i\phi_3} & be^{i\phi_2} & ae^{i\phi_1} & a \end{pmatrix} \tag{III.20}$$

$$\text{with } b = \sqrt{1/2 - a^2},$$

is unitary if

$$\begin{cases} \cos(\phi_2 - \phi_3) = -\dfrac{a^2}{1/2 - a^2}\cos\phi_1 \\ (\phi_2 + \phi_3) = \pi + \phi_1 \end{cases}. \tag{III.21}$$

So that, for given a, we have a one-parameter ambiguity depending on ϕ_1.

However, the discrete ambiguities are reduced. This can be seen from Eq. (III.11), which now becomes a 6th degree equation, because $\varepsilon = \nu$, $T_1 = U_1$ and $R_2 = r_2$. Therefore, outside the continuous ambiguities (which survive in classes B) and C)), there are at most *six* distinct solutions when $U = U^T$.

3. When the matrix of *moduli* is symmetric (without requiring $U = U^T$), the class A) still contains ambiguous configurations with arbitrarily small off-diagonal moduli. Of course, these ambiguities disappear when one sets $\beta = \gamma$ (i.e. in the fully symmetric case), as they should according to Theorem 1.

IV. Discussion

In investigating the case of non-symmetric matrices we have now the surprise of continuous ambiguities, which may exist even if the matrix is close to unity. We have also found examples of continuous ambiguities for symmetric matrices, but however not for matrices close to unity. On the other hand, under condition (II.24) we find that $2^{(n(n-3))/2}$ solutions exist for the symmetric case, and this fits with the results of Ref. [16] where 4 solutions are found. It is tempting to believe that if a unitary matrix is not too far from being symmetric, then under certain conditions, like (II.24), the number of solutions might be the same as for the symmetric case. This is supported by two results:

i) the semi-analytic calculations of Lavoura, for 4×4 matrices, who finds precisely 4 solutions and no more in his examples.

ii) The approximate construction of Bjorken [18] for $n \times n$ matrices, which is done under the condition that the moduli of the matrix have a structure *à la* Wolfenstein.

i) The Lavoura results.
Lavoura [16] gives himself the squares of the moduli of the matrix elements:

$$(|U_{jk}|^2) = \begin{pmatrix} .95 & .0484 & .0001 & .0015 \\ .0489 & .9460 & .0024 & .0027 \\ .0005 & .0040 & .5000 & .4955 \\ .0006 & .0016 & .4975 & .5003 \end{pmatrix}. \tag{IV.1}$$

He gets, for the phases in degrees:

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 179.89 & -25.04 & -173.86 \\ 0 & -74.73 & -137.18 & 138.04 \\ 0 & 73.54 & 117.45 & -147.55 \end{pmatrix}, \tag{IV.2a}$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 179.59 & 160.04 & -123.19 \\ 0 & -103.22 & 23.84 & 156.92 \\ 0 & -8.69 & -144.28 & 168.53 \end{pmatrix} \tag{IV.2b}$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 179.58 & 165.58 & -122.72 \\ 0 & -32.74 & 168.09 & 167.15 \\ 0 & -123.78 & -20.18 & 159.16 \end{pmatrix}, \tag{IV.2c}$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 179.51 & -160.69 & -123.21 \\ 0 & -42.71 & -169.52 & 156.83 \\ 0 & -133.88 & 21.95 & 168.61 \end{pmatrix}. \tag{IV.2d}$$

These results, naturally, do not allow one to draw general conclusions, but they are, nevertheless, very interesting.

ii) The Bjorken approximate construction
In order to construct the KM matrix approximately, Bjorken has invented an iterative method in which unknown contributions can be neglected if the matrix has a structure à la Wolfenstein [19], i.e. if

$$\begin{cases} \left.\begin{matrix} |U_{i,j+1}| \ll |U_{ij}| \\ |U_{i-1,j}| \ll |U_{ij}| \end{matrix}\right\} & \text{for} \quad j \geqq i \\ \left.\begin{matrix} |U_{i,j-1}| \ll |U_{ij}| \\ |U_{i+1,j}| \ll |U_{ij}| \end{matrix}\right\} & \text{for} \quad j \leqq i \end{cases}. \tag{IV.3}$$

In other words, matrix elements decrease very fast as one goes away from the main diagonal of the matrix. This condition is not exactly satisfied by the Lavoura example, in which $|U_{14}|$ is larger than $|U_{34}|$.

Here we shall present the revised version, following a correction by one of us (A.M.). Bjorken makes the following phase convention:

$$U_{ii}\ \text{real} > 0 \quad U_{i,i+1} \geqq 0. \tag{IV.4}$$

Notice that this convention is *not* in agreement with the one made for the symmetric case, so that if the KM matrix were symmetric, the solution obtained by the Bjorken method would not look symmetric and a redefinition of the phases of the lines and the columns would be needed to restore the symmetry.

Under the above assumption,

$$U_{ii} \approx 1, \tag{IV.5}$$

since

$$1 = \sum_i |U_{ij}|^2 = |U_{ii}|^2 + \sum_i{}' |U_{ij}|^2, \tag{IV.6}$$

where $\sum'$ represents the summation over i, $i \neq j$, i.e. over off-diagonal elements.

Then the exact unitarity condition becomes, for $i<j$

$$U_{ji}^* + U_{ij} \cong -\sum_{k=i+1}^{k=j-1} U_{ik} U_{jk}^*. \tag{IV.7}$$

If the matrix element U_{kl} are known for $|k-l| \leqq p$, the right-hand side of (IV.7) can be calculated for $|i-j| \leqq p+1$. Then we have the problem of reconstructing a triangle in the complex plane knowing one side (the right-hand side of (IV.7)), and the length of the two other sides. This problem has *two* or *zero* solutions depending on whether triangular inequalities are satisfied or not.

In the first step of the construction, one gets the elements of the two diagonals, and Eq. (IV.7) reduces to

$$U_{i+1,i}^* + U_{i,i+1} \cong 0 \tag{IV.8}$$

so that, with the phase convention chosen

$$U_{i+1,i} \cong -U_{i,i+1}. \tag{IV.9}$$

If no obstacle is met in this iteration solution, i.e. if all triangular inequalities are satisfied, one gets $2^{(n^2-3n)/2}$ solutions, i.e. exactly the same number as in the symmetric case if condition (II.24) is satisfied. In particular we get 4 solutions for $n=4$.

Now there are two problems.

i) Can we find sufficient conditions so that Bjorken's iterative construction is never blocked by triangular inequalities?

ii) Are Bjorken's "approximate" solutions really approximate? Is there a one-to-one correspondence between an approximate solution and a true solution?

To problem i) we can give an answer which, crudely speaking, is that we should have on the one hand conditions analogous to (II.24) for the symmetric case and on the other hand the antisymmetric part of the matrix should be "very small" compared to the symmetric part.

First we must satisfy

$$|U_{ji}| + |U_{ij}| > |\textstyle\sum' U_{ik} U_{jk}^*|. \tag{IV.10}$$

This will be true if we have the *sufficient* condition

$$|U_{ji}| + |U_{ij}| > \sum_{i_> < k_> < j} |U_{ik}||U_{jk}|, \tag{IV.11}$$

but we need also

$$||U_{ji}|-|U_{ij}||<\left|\sum_{i_{>}<k_{>}<j} U_{ik}U_{jk}^{*}\right| \tag{IV.12}$$

and it is difficult to find a way to ensure this with a condition involving only the moduli, except if one term is dominating in the right-hand side of (IV.12). So a sufficient condition will be

$$||U_{ji}|-|U_{ij}||< 2\sup_{i_{>}<k_{>}<j}|U_{ik}||U_{jk}|-\sum_{i_{>}<k_{>}<j}|U_{ik}||U_{jk}|. \tag{IV.13}$$

For $n=4$ the right-hand side of (IV.13) is always positive or, exceptionally, zero, because $\sum$ is at most made of 2 terms (when $i=1$ and $j=4$ or $i=4$ and $j=1$).

For $n \geqq 5$ one procedure to ensure the positivity of the right-hand side of (IV.13) is to take

$$|U_{ij}| \cong \lambda c_{ij}\varepsilon^{|i-j|^2}, \quad \varepsilon<1, \tag{IV.14}$$

instead of

$$|U_{ij}| \cong c_{ij}\varepsilon^{|i-j|}, \tag{IV.15}$$

which is the Wolfenstein–Bjorken case.

A strategy to construct examples of moduli leading to the $2^{(n^2-3n)/2}$ approximate solutions is to take a symmetric matrix of the squares of the moduli of the form $\lambda a_{ij}\varepsilon^{|i-j|^2}$, $a_{ij}\neq 0$.

Take ε sufficiently small to ensure that all right-hand sides of (IV.13) are *strictly* positive, then take λ small enough so that inequalities (IV.11) are satisfied. Then one can add to the matrix of the squares of the moduli an antisymmetric matrix μA_{ij}. For μ sufficiently small, inequalities (IV.13) will be satisfied and also inequalities (IV.11) for which the antisymmetric part is a small perturbation.

In conclusion, one can invent scenarios in which the matrix of the moduli is such that all $2^{(n^2-3n)/2}$ approximate solutions exist (here we do not count the complex conjugation of U!).

The question whether there is a relationship between approximate and exact solutions is very difficult. It would be tempting to use the Bjorken solution as the starting point of an iterative scheme, the first step being to use the Bjorken solution in $\sum U_{jk}^{*}U_{ik}$, without neglecting the "small" terms. Then, at the end of the first step the phase convention would be destroyed and the matrix should be "renormalized" before starting again. There is, unfortunately, no indication that this scheme converges, as far as we can see at the present time.

One could ask under which conditions an iterative scheme

$$U^{p}\rightarrow U^{p+1},$$

where

$$U_{ii}U_{ji}^{*p+1}+U_{ij}^{p+1}U_{jj}^{*}=-\sum_{k}{}' U_{ik}^{p}U_{jk}^{*p} \tag{IV.16}$$

is not blocked by triangular constraints. Sufficient conditions, analogous to the previous ones can be found:

$$|U_{ii}||U_{ji}|+|U_{jj}||U_{ji}|>\sum{}'|U_{ik}||U_{jk}| \tag{IV.17}$$

and

$$||U_{ii}||U_{ji}|-|U_{jj}||U_{ji}||+\sum{}'|U_{ik}||U_{jk}| \quad <2\sup_{\substack{k\neq i\\ k\neq j}}|U_{ik}||U_{jk}|. \tag{IV.18}$$

Again the set of matrices satisfying these conditions is *not empty*, but we do not know if the iteration converges (modulo a redefinition of the phases at each step), and we cannot use a Leray–Schauder argument to prove at least the existence of solutions, because we lack "convexity" properties. This does not mean that the problem cannot be solved, but that it is difficult!

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