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First determination of the Jarlskog invariant of CP violation from the moduli of the CKM matrix elements

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ABSTRACT

We find that the precision and accuracy of current experimental data on the moduli of nine Cabibbo-Kobayashi-Maskawa (CKM) quark flavor mixing matrix elements allow us to numerically determine the *correct* size of the Jarlskog invariant of CP violation from four of them in eight different ways *for the first time* without making any special assumptions. This observation implies a remarkable self-consistency of the correlation between CP-conserving and CP-violating quantities of the CKM matrix as guaranteed by its unitarity.

1. Introduction

In the standard model (SM) of particle physics, the phenomena of quark flavor mixing and weak CP violation are elegantly described by a nontrivial 3×3 unitary matrix appearing in the flavor-changing charged-current interactions, the well-known Cabibbo-Kobayashi-Maskawa (CKM) matrix V [1,2]. The unitarity of V, which can be expressed as a combination of the normalization and orthogonality conditions (for $\alpha, \beta = u, c, t$ and $i, j = d, s, b$)

$$\sum_i V_{\alpha i} V^*_{\beta i} = \delta_{\alpha\beta} \, , \qquad \sum_\alpha V_{\alpha i} V^*_{\alpha j} = \delta_{ij} \, , \tag{1}$$

is the only but powerful constraint imposed by the SM itself. In particular, this constraint leads us to a unique rephasing-invariant measure of CP violation in the quark sector — the so-called Jarlskog invariant $\mathcal{J}$ [3,4] defined through

$$\mathrm{Im}\left(V_{\alpha i} V_{\beta j} V^*_{\alpha j} V^*_{\beta i}\right) = \mathcal{J} \sum_\gamma \epsilon_{\alpha\beta\gamma} \sum_k \epsilon_{ijk} \, , \tag{2}$$

where $\epsilon_{\alpha\beta\gamma}$ and ϵ_{ijk} denote the three-dimensional Levi-Civita symbols with the Greek and Latin subscripts running respectively over (u, c, t) and (d, s, b). As the moduli of nine CKM matrix elements are also rephasing-invariant, Eqs. (1) and (2) give rise to a rather striking correlation between the CP-violating and CP-conserving invariants of V [5,6]:

$$\mathcal{J}^2 = |V_{\alpha i}|^2 |V_{\beta j}|^2 |V_{\alpha j}|^2 |V_{\beta i}|^2 - \frac{1}{4}\left(|V_{\alpha i}|^2 |V_{\beta j}|^2 + |V_{\alpha j}|^2 |V_{\beta i}|^2 - |V_{\gamma k}|^2\right)^2 \, , \tag{3}$$

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where $\alpha \neq \beta \neq \gamma$ and $i \neq j \neq k$ are certainly required. One may in principle use this algebraic relation to calculate the size of $\mathcal{J}$ from any four independent moduli of the CKM matrix elements, and then compare the result with the value of $\mathcal{J}$ extracted from the CP-violating asymmetries in some hadronic decay modes (e.g., an asymmetry between the rates of B_d^0 and $\bar{B}_d^0 \to J/\psi + K_S$ decays [7]). Such a test of the validity of Eq. (3) with the relevant experimental data makes sense because it offers another viable way to cross check the unitarity of V.

But Eq. (3) has never been successfully confronted with the available experimental data in the past decades.[1] The main reason is simply that the expression of $\mathcal{J}^2$ is a difference between two positive terms consisting of a number of moduli of the CKM matrix elements. So the positivity and smallness of $\mathcal{J}^2$ implies that its first term must be slightly larger than its second term, and a significant cancellation between these two terms is in general unavoidable. In this case the input values of all the CP-conserving quantities on the right-hand side of Eq. (3) must be as precise as possible and maximally compatible with the unitarity conditions of V, otherwise the output value of $\mathcal{J}^2$ would be either negative or in conflict with the result of $\mathcal{J}$ determined from CP violation in B and K decays. Then the question arises: can today's experimental measurements of the CKM matrix elements allow us to reliably calculate the size of $\mathcal{J}$ from Eq. (3)?

The answer is affirmative, but it depends highly on which four independent $|V_{\alpha i}|$ (for $\alpha = u, c, t$ and $i = d, s, b$) are taken into account. In this article we are going to show that, *for the first time*, the correct size of the Jarlskog invariant of CP violation can be numerically calculated from the moduli of the CKM matrix elements with the available experimental data and without making any special assumptions. We find that there are eight different ways to do so for the time being, and they all include the moduli of the two smallest CKM matrix elements $|V_{ub}|$ and $|V_{td}|$.

2. How good are the data of $|V_{\alpha i}|$ to fit unitarity?

To clearly see the fine difference between any two of the CKM matrix elements with a comparable magnitude, let us adopt the Wolfenstein-like expansion of V as follows [9,10]:

$$
\begin{aligned}
V_{ud} &= 1 - \frac{1}{2}\lambda^2 - \frac{1}{8}\lambda^4 + \mathcal{O}(\lambda^6)\,, \\
V_{us} &= \lambda + \mathcal{O}(\lambda^7)\,, \\
V_{ub} &= A\lambda^3(\rho - \mathrm{i}\eta)\;; \\
V_{cd} &= -\lambda + \frac{1}{2}A^2\lambda^5\left[1 - 2(\rho + \mathrm{i}\eta)\right] + \mathcal{O}(\lambda^7)\,, \\
V_{cs} &= 1 - \frac{1}{2}\lambda^2 - \frac{1}{8}\lambda^4\left(1 + 4A^2\right) + \mathcal{O}(\lambda^6)\,, \\
V_{cb} &= A\lambda^2 + \mathcal{O}(\lambda^8)\,; \\
V_{td} &= A\lambda^3(1 - \rho - \mathrm{i}\eta) + \frac{1}{2}A\lambda^5(\rho + \mathrm{i}\eta) + \mathcal{O}(\lambda^7)\,, \\
V_{ts} &= -A\lambda^2 + \frac{1}{2}A\lambda^4\left[1 - 2(\rho + \mathrm{i}\eta)\right] + \mathcal{O}(\lambda^6)\,, \\
V_{tb} &= 1 - \frac{1}{2}A^2\lambda^4 + \mathcal{O}(\lambda^6)\,,
\end{aligned} \tag{4}
$$

where $V_{ub} = A\lambda^3(\rho - \mathrm{i}\eta)$ is exact by definition, λ denotes the small expansion parameter, and the unitarity of V is valid at the level of $\mathcal{O}(\lambda^6)$. Current experimental data [7] lead us to $\lambda \simeq 0.225$, $A \simeq 0.825$, $\rho \simeq 0.163$ and $\eta \simeq 0.357$ in the neglect of their corresponding error bars. Then we can easily arrive at a remarkable ordering for the nine elements of V, as first observed in Ref. [11]:

$$
\begin{aligned}
|V_{tb}| > |V_{ud}| > |V_{cs}| \gg |V_{us}| > |V_{cd}| & \\
\gg |V_{cb}| > |V_{ts}| & \\
\gg |V_{td}| > |V_{ub}|\,. &
\end{aligned} \tag{5}
$$

In comparison, the present experimental values of nine moduli of V are [7]

$$
\begin{pmatrix} |V_{ud}| & |V_{us}| & |V_{ub}| \\ |V_{cd}| & |V_{cs}| & |V_{cb}| \\ |V_{td}| & |V_{ts}| & |V_{tb}| \end{pmatrix} = \begin{pmatrix} 0.97373 \pm 0.00031 & 0.2243 \pm 0.0008 & (3.82 \pm 0.20) \times 10^{-3} \\ 0.221 \pm 0.004 & 0.975 \pm 0.006 & (40.8 \pm 1.4) \times 10^{-3} \\ (8.6 \pm 0.2) \times 10^{-3} & (41.5 \pm 0.9) \times 10^{-3} & 1.014 \pm 0.029 \end{pmatrix}. \tag{6}
$$

Some immediate comments are in order.

[1] A preliminary attempt was made to calculate $\mathcal{J}$ from the inputs of $|V_{us}|$, $|V_{cd}|$, $|V_{ub}|$ and $|V_{cb}|$ in Ref. [8], with a conclusion that "it is not feasible *in practice*". The authors assumed the Gaussian probability density distributions around the central values of the moduli of these four CKM matrix elements, and adopted a toy Monte Carlo method to compute the probability density distribution of $\mathcal{J}^2$. They found that only 7.9% of the generated points could assure the positivity of $\mathcal{J}^2$, unfortunately.

- The experimental values of $|V_{ub}|$ and $|V_{td}|$ confirm that they are the two smallest moduli of the CKM matrix elements and in the correct ordering. It will therefore be safe to choose these two moduli to calculate the magnitude of the Jarlskog invariant $\mathcal{J}$ with the help of Eq. (3), as their impacts on the normalization conditions of V are negligible in most cases.
- The central values of $|V_{cb}|$ and $|V_{ts}|$ imply that they seem to be in a wrong ordering, in conflict with the expectation shown in Eq. (5) as required by the unitarity of V. So a further improvement of the precision and accuracy associated with the individual measurements of $|V_{cb}|$ and $|V_{ts}|$ is no doubt necessary.
- The fact that $|V_{us}|$ should be slightly larger than $|V_{cd}|$ has essentially been established from today's data, as one can see from Eq. (6). A precision measurement of $|V_{cd}|$ in the near future may more convincingly strengthen this observation.
- The central values of $|V_{ud}|$ and $|V_{cs}|$ imply that they seem to be in an ordering inconsistent with the expectation from Eq. (5). The reason is simply that there remain some quite large uncertainties associated with the determination of $|V_{cs}|$. As both $|V_{ud}|$ and $|V_{cs}|$ are close to one, their errors may easily invalidate the normalization conditions of V in some cases.
- The value of $|V_{tb}|$ involves the largest uncertainty and is apparently incompatible with the unitarity requirement of V, although it looks like the largest moduli as expected among the nine moduli of the CKM matrix elements. So one should better avoid using the present experimental result of $|V_{tb}|$ to calculate $\mathcal{J}^2$ via Eq. (3).

In short, $|V_{ub}|$ and $|V_{td}|$ should be taken into account when combining Eq. (3) and Eq. (6) to calculate $\mathcal{J}$. Whether such a calculation can successfully lead us to a meaningful result of $\mathcal{J}$ depends on whether the input values of the other two independent moduli of the CKM matrix elements are accurate enough and maximally consistent with the unitarity conditions. Let us make things clear by checking all the possibilities along this line of thought.

3. Calculations of $|\mathcal{J}|$ from the moduli of $V_{\alpha i}$

It is straightforward to figure out that there are totally $C_9^4 = 9!/(4!\,5!) = 126$ possibilities to randomly choose any four of the nine CKM matrix elements, but 45 of them should be abandoned since the chosen four matrix elements are not completely independent. To be more specific, we find that the possibilities in the following two categories ought to be eliminated.

- If three of the four chosen CKM matrix elements lie in the same row or column of V, they must satisfy the corresponding normalization condition and thus are not fully independent. There are totally 6×6 possibilities belonging to this category, where the first "6" means a sum of three possible rows and three possible columns, and the second "6" indicates that the fourth CKM matrix element may be any of the other six CKM matrix elements which is located in a different row or column.
- If two of the four chosen CKM matrix elements lie in a row of V and the other two lie in a column of V except the possibilities that three of them are located in the same row or column, then they must not be fully independent. For example, V_{us} and V_{ub} in the first row are related to V_{cd} and V_{td} in the first column via $|V_{us}|^2 + |V_{ub}|^2 = |V_{cd}|^2 + |V_{td}|^2$. There are totally 9 possibilities of this category.

As a result, we are left with $126 - 36 - 9 = 81$ different ways of choosing a set of four independent CKM matrix elements. We find that these 81 possibilities can be categorized into the following three different groups.

- The four chosen CKM matrix elements are independent and located in *two* rows and *two* columns of V, such as the patterns
$$\begin{pmatrix} \times & \times & \\ \times & \times & \\ & & \end{pmatrix}, \quad \begin{pmatrix} \times & & \times \\ \times & & \times \\ & & \end{pmatrix}, \quad \begin{pmatrix} \times & \times & \\ & & \\ \times & \times & \end{pmatrix}. \tag{7}$$
There are totally 9 different patterns of this category.
- The four chosen CKM matrix elements are independent and located in *two* rows and *three* columns (or *two* columns and *three* rows) of V, such as the patterns
$$\begin{pmatrix} \times & \times & \\ \times & & \times \\ & & \end{pmatrix}, \quad \begin{pmatrix} \times & & \times \\ & & \\ \times & \times & \end{pmatrix}, \quad \begin{pmatrix} \times & \times & \\ \times & & \\ & \times & \end{pmatrix}. \tag{8}$$
There are totally 36 different patterns of this category.
- The four chosen CKM matrix elements are independent and located in *three* rows and *three* columns of V, such as the patterns
$$\begin{pmatrix} \times & \times & \\ \times & & \\ & & \times \end{pmatrix}, \quad \begin{pmatrix} \times & & \times \\ & \times & \\ \times & & \end{pmatrix}, \quad \begin{pmatrix} \times & & \times \\ \times & & \\ & \times & \end{pmatrix}. \tag{9}$$
There are totally 36 different patterns of this category.

As pointed out in section 2, the values of some of the moduli of the nine CKM matrix elements involve quite large uncertainties and may not respect the unitarity conditions to a good degree of accuracy when they are input to calculate $\mathcal{J}^2$ from Eq. (3). In this case the output of $\mathcal{J}^2$ is likely to be either negative or too far away from the global fit result $\mathcal{J} = \left(3.08^{+0.15}_{-0.13}\right) \times 10^{-5}$ advocated by the Particle Data Group [7].

We proceed to do a careful numerical analysis of all the aforementioned 81 possibilities of choosing the four independent CKM matrix elements and calculating $\mathcal{J}^2$ from Eq. (3) by adopting a strategy as follows. Given the very fact that the errors of $|V_{\alpha i}|$ (for $\alpha = u, c, t$ and $i = d, s, b$) listed in Eq. (6) involve some theoretical uncertainties which do not really obey the Gaussian probability density distributions [7], we simply make a random scan within the given error bar for each of the nine $|V_{\alpha i}|$ instead of assuming any particular statistical distributions regarding the uncertainties of $|V_{\alpha i}|$. This conservative strategy may largely assure that the correct output of $\mathcal{J}^2$ is not fragile in the sense that it is essentially stable even when a particular probability density distribution around the central value of $|V_{\alpha i}|$ is assumed (but the reverse may not be true, as we have checked). After some lengthy calculations, we find that current data on $|V_{\alpha i}|$ only allow the following eight choices to be viable.

- The four independent CKM matrix elements are V_{ud}, V_{ub}, V_{td} and V_{cb} or V_{ts}:

$$\begin{pmatrix} V_{ud} & & V_{ub} \\ & & V_{cb} \\ V_{td} & & \end{pmatrix}, \quad \begin{pmatrix} V_{ud} & & V_{ub} \\ & & \\ V_{td} & V_{ts} & \end{pmatrix}, \tag{10}$$

  from which the results $\mathcal{J} = \left(3.20^{+0.25}_{-0.28}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.19^{+0.25}_{-0.32}\right) \times 10^{-5}$ can be respectively obtained.[2]
  Here the central value of $\mathcal{J}$ is achieved from the central values of the four input moduli, and its upper and lower bounds correspond to its maximal and minimal values extracted from our random scans within the given error bars of the relevant moduli.
- The four independent CKM matrix elements are V_{us}, V_{ub}, V_{td} and V_{cb} or V_{ts}:

$$\begin{pmatrix} & V_{us} & V_{ub} \\ & & V_{cb} \\ V_{td} & & \end{pmatrix}, \quad \begin{pmatrix} & V_{us} & V_{ub} \\ & & \\ V_{td} & V_{ts} & \end{pmatrix}, \tag{11}$$

  from which the numerical results $\mathcal{J} = \left(3.19^{+0.25}_{-0.25}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.20^{+0.25}_{-0.29}\right) \times 10^{-5}$ can be respectively achieved.
- The four independent CKM matrix elements are V_{cd}, V_{ub}, V_{td} and V_{cb} or V_{ts}:

$$\begin{pmatrix} & & V_{ub} \\ V_{cd} & & V_{cb} \\ V_{td} & & \end{pmatrix}, \quad \begin{pmatrix} & & V_{ub} \\ V_{cd} & & \\ V_{td} & V_{ts} & \end{pmatrix}, \tag{12}$$

  from which $\mathcal{J} = \left(3.19^{+0.26}_{-0.26}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.20^{+0.24}_{-0.29}\right) \times 10^{-5}$ can be respectively obtained.
- The four independent CKM matrix elements are V_{cs}, V_{ub}, V_{td} and V_{cb} or V_{ts}:

$$\begin{pmatrix} & & V_{ub} \\ & V_{cs} & V_{cb} \\ V_{td} & & \end{pmatrix}, \quad \begin{pmatrix} & & V_{ub} \\ & V_{cs} & \\ V_{td} & V_{ts} & \end{pmatrix}, \tag{13}$$

  from which $\mathcal{J} = \left(3.18^{+0.27}_{-0.55}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.20^{+0.25}_{-0.58}\right) \times 10^{-5}$ can be respectively achieved.

The most salient and common feature of these eight patterns is that they all include the two smallest CKM matrix elements V_{ub} and V_{td} of $\mathcal{O}(\lambda^3)$, besides one of the CKM matrix elements of $\mathcal{O}(\lambda^2)$ (i.e., V_{cb} or V_{ts}). In any of the above eight choices, the fourth CKM matrix element can be either V_{ud} (or V_{cs}) of $\mathcal{O}(1)$ or V_{us} (or V_{cd}) of $\mathcal{O}(\lambda)$. As expected, the possibilities associated with the largest CKM matrix element V_{tb} have been excluded from our calculations simply because the present value of $|V_{tb}|$ is most "unitarity-unfriendly". One may also see that the outputs of $\mathcal{J}$ involve a bit larger error bars in Eq. (13) as compared with those in Eqs. (10)—(12), since the input value of $|V_{cs}|$ remains "unitarity-unsatisfactory".

At this point one may expect that the allowed range of $\mathcal{J}$ in each of the above eight cases should more or less be narrowed, if the additional constraints $|V_{td}/V_{ts}| = 0.207 \pm 0.004$ and $|V_{ub}/V_{cb}| = 0.084 \pm 0.007$ [7] are taken into account together with Eq. (6). We confirm that this expectation is true, and obtain $\mathcal{J} = \left(3.20^{+0.25}_{-0.28}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.19^{+0.25}_{-0.27}\right) \times 10^{-5}$ for the two patterns in Eq. (10); $\mathcal{J} = \left(3.19^{+0.25}_{-0.25}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.20^{+0.25}_{-0.26}\right) \times 10^{-5}$ for the two patterns in Eq. (11); $\mathcal{J} = \left(3.19^{+0.26}_{-0.25}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.20^{+0.24}_{-0.26}\right) \times 10^{-5}$ for the two patterns in Eq. (12); $\mathcal{J} = \left(3.18^{+0.27}_{-0.52}\right) \times 10^{-5}$ and $\mathcal{J} = \left(3.20^{+0.25}_{-0.47}\right) \times 10^{-5}$ for the two patterns in Eq. (13). In particular, the lower bound of $\mathcal{J}$ is more sensitive to the constraint $|V_{td}/V_{ts}|$.

[2] We have abandoned the respective solutions $\mathcal{J} = -\left(3.20^{+0.25}_{-0.28}\right) \times 10^{-5}$ and $\mathcal{J} = -\left(3.19^{+0.25}_{-0.32}\right) \times 10^{-5}$ that are mathematically allowed by Eq. (3), simply because $\mathcal{J} > 0$ has been experimentally established on solid ground [7].

4. Summary

The usefulness of the Jarlskog invariant $\mathcal{J}$ as a rephasing-independent measure of weak CP violation has been well recognized in both the quark sector and the lepton sector.[3]

It is also known that $\mathcal{J}$ can be expressed in terms of any four independent moduli of the nine quark or lepton flavor mixing matrix elements, as guaranteed by the unitarity conditions. This kind of correlation between the CP-violating and CP-conserving quantities should be experimentally tested, as it can provide a novel way to cross check the unitarity of the CKM or PMNS matrix.

We have shown that, *for the first time*, the correct size of the Jarlskog invariant of CP violation can be numerically calculated from the moduli of the CKM matrix elements with the help of the currently available experimental data and without making any special assumptions. But we find that there are only eight different ways to do so, as limited by the precision and accuracy of the relevant experimental values of $|V_{\alpha i}|$ (for $\alpha = u, c, t$ and $i = d, s, b$). This encouraging observation implies that the unitarity of the CKM matrix deserves a further and more reliable test in the upcoming precision measurement era of flavor physics characterized by the High-Luminosity Large Hadron Collider. The same expectation makes sense for testing the unitarity of the 3×3 PMNS matrix and constraining possible extra species of massive neutrinos in the precision measurement era of neutrino physics.[4]

CRediT authorship contribution statement

Shu Luo: Investigation, Methodology, Writing – original draft, Writing – review & editing. **Zhi-zhong Xing:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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[3] This will be true if the 3×3 Pontecorvo-Maki-Nakagawa-Sakata (PMNS) lepton flavor mixing matrix [12–14] is assumed to be exactly unitary. The early discussions about leptonic CP violation in a 3×3 unitary flavor mixing matrix can be found in Ref. [15] and especially in Ref. [16].

[4] The possibility of determining the Jarlskog invariant of leptonic CP violation from the three CP-conserving quantities in $\nu_\mu \to \nu_e$ and $\overline{\nu}_\mu \to \overline{\nu}_e$ oscillations has recently been discussed by us [17].