

Efficient Identification the Inequivalence of Mutually Unbiased Bases via Finite Operators

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The structural characterization of high-dimensional mutually unbiased bases (MUBs) by classifying MUBs subsets remains a major open problem. The existing methods not only fail to conclude on the exact classification, but also are severely limited by computational resources and suffer from the numerical precision problem. Here we introduce an operational approach to identify the inequivalence of MUBs subsets, which has less time complexity and entirely avoids the computational precision issues. For arbitrary MUBs subsets of k elements in any prime dimension, this method yields a universal analytical upper bound for the amount of MUBs equivalence classes. By applying this method through simple iterations, we further obtain tighter classification upper bounds for any prime dimension $d \leq 37$. Crucially, the comparison of these upper bounds with existing lower bounds successfully determines the exact classification for all MUBs subsets in any dimension $d \leq 17$. We further extend this method to the case that the dimension is a power of prime number. This general and scalable framework for the classification of MUBs subsets sheds new light on related applications.

Introduction.— Incompatible measurements are the cornerstones of quantum information theory and techniques. As the “maximally incompatible” measurements [1–4], mutually unbiased bases (MUBs) plays a crucial role in quantum tasks such as quantum state tomography [5–13], quantum key distribution [14–19], quantum random number generation [20–22] and detection of quantum nonlocality [23–29].

In a d -dimensional Hilbert space, two orthonormal bases $\{|e_i\rangle\}$ and $\{|f_j\rangle\}$ are called MUBs if $|\langle e_i|f_j\rangle|^2 = 1/d$ for all i, j . One main research line on this topic is to understand the structure of MUBs, such as determining the maximum amount of MUBs in a given dimension. Such a question has been solved constructively for the prime-power dimension d , where the the maximum amount of MUBs is $d + 1$. However, even when d is the simple composite number 6, it is still an open question after decades of research [30–34]. In Parallel, a new perspective to explore the MUB structures is from determining the inequivalence classes of subsets of k MUBs. Two subsets of k MUBs are equivalent if and only if one subset can be transformed into another one by operations including unitary rotations, complex conjugation, global phases, column permutations, and reordering of bases [35–38]. In high dimensions ($d \geq 5$), MUBs subsets are known to exhibit multiple inequivalence classes [39–45]. While, direct classification by definition is impractical, as it requires exploring an uncountable set of operations. To address this, the operational criterion based on Shannon entropy [40, 46–53], robustness of incompatible measurements [41, 42, 54], accuracy of quantum random access code [43], entanglement detection efficiency [44], and diamond distance [45, 55, 56] have been proposed. Since those criteria are only sufficient conditions for the inequivalent classes, they generally provide only the lower bounds of the amount of classes in the classification. It is not known whether any criterion exactly characterize the classification. More importantly, as the dimension

of the system or the size of the subsets increases, those numerical methods encounter the following obstacles: (i) optimization procedures easily get trapped in local optima instead of the global one, e.g., the criterion based on Shannon entropy is a non-convex programming; (ii) the distinction between the values of different classes are so subtle that the resulting classification might be spurious; (iii) the requirement of computational resources goes beyond the available capacity quickly as the dimension of the system and the size of subsets increases.

In this work, we proposes an analytical method to classify MUBs subsets based on finite transformation group. By using a subset of those operations, we first derive a universal upper bound for the amount of inequivalent classes of MUBs subsets in any prime dimension d , which yields the exact classification for $d = 5$. A further systematical application of this method leads to a more tight upper bound on the amount of inequivalent classes for any other prime dimension $d \leq 37$. Critically, such an upper bound coincides with the lower bound derived from the Shannon entropy criterion, and thus successfully determines the exact classification for all MUBs subsets of any size k in prime dimension $d \leq 17$, and cases of small k for higher dimension d . The method is also generalized for prime-power dimensions by incorporating more transformations, which results in the exact classification for dimension $d = 9$. Finally, complexity analysis and practical performance reveal that this approach is computationally lighter than the existing methods.

MUBs classification using finite unitary matrices.— In a Hilbert space of prime dimension d , there exists a complete set of $d + 1$ MUBs [1, 2], denoted as $\mathcal{M} = \{M_0, \dots, M_d\}$. Any element M_x in the set of MUBs is composed of d complete

orthonormal basis vectors $\{|\psi_{a,x}\rangle\}$, which can be defined as

$$|\psi_{a,x}\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \omega^{xj^2 - aj} |j\rangle, \quad x \in \{0, 1, \dots, d-1\},$$

$$|\psi_{a,d}\rangle = \sum_{j=0}^{d-1} \delta_{j,a} |j\rangle, \quad x = d, \quad (1)$$

where $|j\rangle$ is computational basis, $\omega = e^{2\pi i/d}$, and $a \in \{0, 1, \dots, d-1\}$. The main task is to determine the exact amount of inequivalence classes formed by arbitrarily selected subsets of k MUBs from this collection for a give positive integer $k \leq d+1$.

Since unitary transformations are arbitrary, it is generally infeasible to distinguish inequivalent MUBs subsets directly from their definition. We define a finite set of unitary transformation matrices containing only $d+1$ elements based on the MUBs set $\mathcal{M}$, denoted as $\mathcal{U}_{\text{finite}} = \{M_0, \dots, M_d\}$. We rigorously prove that any operation M_x within this finite unitary set $\mathcal{U}_{\text{finite}}$ possesses a crucial closure property: it transforms the orthonormal basis vectors $|\psi_{b,y}\rangle$ of any y -th MUB into the basis vectors $|\psi_{c,z}\rangle$ of the z -th MUB within the complete set $\mathcal{M}$. This establishes a one-to-one correspondence ($y \rightarrow z$) among the MUB indices for a fixed M_x . Specifically, when $x = d$, M_d is the identity matrix, and the basis vectors $\{|\psi_{b,y}\rangle\}$ remain unchanged. For $x \in \{0, 1, \dots, d-1\}$ and $y \in \{1, \dots, d-1\}$, the new basis vector indices satisfy the exact analytic relations $\{z = x - \frac{1}{4y} \pmod{d}, \quad c = \frac{b}{2y} \pmod{d}\}$. Specifically, when $y = 0$, any M_x transforms the basis vectors $\{|\psi_{b,0}\rangle\}$ into the computational basis vectors. When $y = d$, the unitary operator M_x transforms $\{|\psi_{b,d}\rangle\}$ into the orthonormal basis vectors corresponding to M_x itself. This explicit, finite, and closed mapping is central to our MUBs classification framework (detailed proof in Sec.II of Supplemental Material(SM)).

Based on this finite set of unitary operations and their tractable transformation, we derive a universal analytical upper bound for the amount of MUBs inequivalence classes.

Theorem 1. *In a prime-dimensional Hilbert space of dimension d , the classification of mutually unbiased bases (MUBs) subsets satisfies the following properties:*

$$N_k \leq \begin{cases} 1, & \text{if } k = 1 \text{ or } d, \\ \frac{\binom{d+1}{k}}{2d}, & \text{if } 1 < k < d. \end{cases} \quad (2)$$

Since there is at least one class, the derived upper bound is saturated in the case that $k = 1$ or $k = d$. For $1 < k < d$, the upper bound is derived by proving that the finite unitary group $\mathcal{U}_{\text{finite}}$, acting on the complete MUBs sets $\mathcal{M}$, generates a minimum of $2d$ inequivalent subsets (orbits). Details of the proof are provided in Sec.III of SM. Crucially, for the first known case of existing multiple inequivalent classes ($d = 5, k = 3$) [41], this upper bound exactly yields $N_{\text{UB}} = \binom{6}{3}/10 = 2$, perfectly matching the known amount of inequivalent classes [39–45]. However, the tightness of this bound

deteriorates rapidly in higher dimensions due to the further overlap of distinct orbits. To achieve a tighter upper bound, we refine our method by incorporating complex conjugation operations into the $\mathcal{U}_{\text{finite}}$ group. Most notably, combining this tighter upper bound with existing lower bounds [41] allows us to achieve, for the first time, the exact classification of MUBs inequivalence classes for dimensions $d \leq 17$.

TABLE I. Transformation table of the finite operations in $d = 5$

$U \backslash M_y$	M_0	M_1	M_2	M_3	M_4	M_5
M_0	5	1	3	2	4	0
M_1	5	2	4	3	0	1
M_2	5	3	0	4	1	2
M_3	5	4	1	0	2	3
M_4	5	0	2	1	3	4
M_5	0	1	2	3	4	5
conj	0	4	3	2	1	5

Determining the Exact Classification for Prime Dimensions based on Upper and Lower Bounds.— Our core methodology determine MUBs inequivalence classes by analyzing transformations under the finite unitary group $\mathcal{U}_{\text{finite}}$ and complex conjugation. Complex conjugation maintains operational equivalence, as any basis vector $|\psi_{b,y}\rangle$ transforms analytically to a vector within the complete set $\mathcal{M}$ via the relation $z = -y \pmod{d}, c = -b \pmod{d}$. This approach is significant because it not only provides bounds on the amount of inequivalent classes but, more importantly, enables the precise identification of their sets.

MUBs Inequivalence Classes Classification Method.— As shown in Fig. 1, this method includes the following three steps:

(1). By traversing all unitary transformations in $\mathcal{U}_{\text{finite}}$ and their complex conjugates, we construct a $(d+2) \times (d+1)$ “Transformation Table”, which records the action on each $M_y \in \mathcal{M}$ and enables efficient indexing for equivalence analysis.

(2). Starting with an initial subset $\mathcal{S} = \{M_1, \dots, M_k\}$, we determine its complete equivalence class $\mathcal{C}$ via an iterative search. The $d+2$ equivalent subsets are rapidly identified using the transformation table. Each newly generated subset is subjected to standardized ordering (ascending by MUB index) to ensure unique representation, stored in the set $\mathcal{C}$ (removing duplicates), and added to the processing queue $\mathcal{Q}$. This procedure is repeated iteratively by selecting subsets from $\mathcal{Q}$ until the queue is exhausted ($\mathcal{Q} = \emptyset$). Then $\mathcal{C}$ fully contains all subsets equivalent to the initial set $\mathcal{S}$.

(3). Defining the initial set $\mathcal{R}$ as the complete collection of $\binom{d+1}{k}$ k -MUBs subsets, the classification proceeds by iteratively selecting an unclassified subset $\mathcal{S}$ from $\mathcal{R}$, generating its complete equivalence class $\mathcal{C}$, and adding $\mathcal{C}$ to the final partition $\mathcal{L}$. All elements of $\mathcal{C}$ are then removed from $\mathcal{R}$. This procedure is repeated until $\mathcal{R} = \emptyset$, yielding $\mathcal{L}$ as the complete classification of all inequivalent k -MUBs subsets.

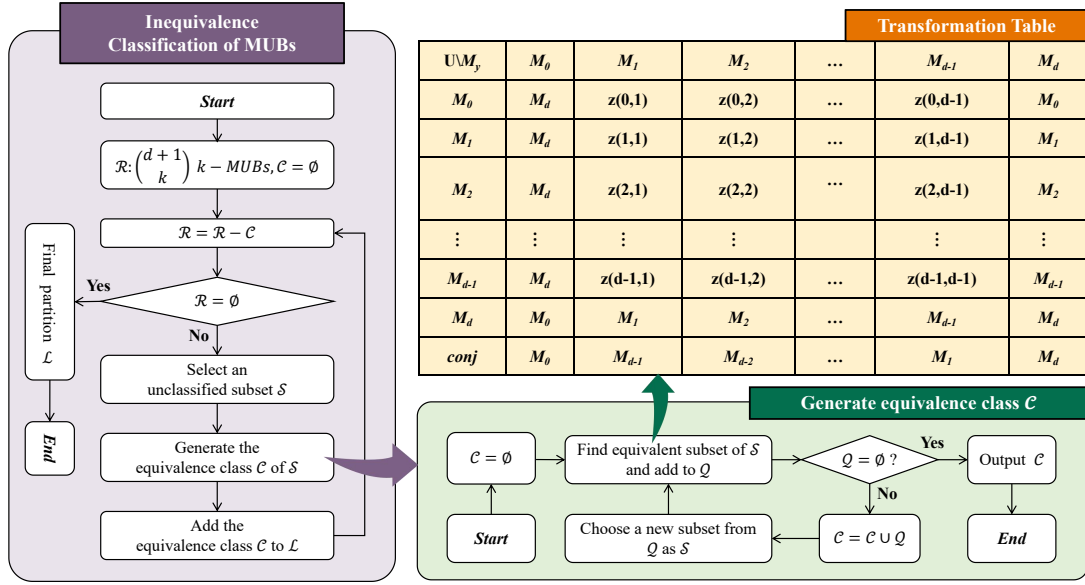


FIG. 1. Schematic of the finite-group classification method. $\mathcal{R}$, $\mathcal{Q}$ and $\mathcal{L}$ represent the unclassified collection, the processing queue and the classified collection, respectively.

As an illustration, consider $d = 5$, where $\mathcal{U}_{\text{finite}} = \{M_0, \dots, M_5\}$. Applying each $U \in \mathcal{U}_{\text{finite}}$ and its conjugate to the full set $\mathcal{M}$ yields the complete “Transformation Table” (Table I). This enables efficient classification: for $k = 2$, all $\binom{6}{2} = 15$ subsets belong to a single equivalence class; for $k = 3$, two inequivalent classes emerge (e.g., $\{M_0, M_1, M_2\}$ and $\{M_0, M_1, M_3\}$). These results fully agree with previous findings [40–44]. Extending this method, we determine both upper bounds and explicit classifications of inequivalent k -MUBs subsets for all prime $d \leq 37$ (see Table II).

Lower bound of Inequivalent MUBs Classes Based on the Shannon Entropy Criterion.— Previous studies on inequivalent MUBs have mainly provided lower bounds using criteria such as robustness of incompatible measurements [41] or the Shannon entropy [40]. Adopting the latter, we classified all subsets for $d \leq 17$ (Table II), which clearly distinguishes inequivalent classes in low dimensions (e.g., $d = 5$, $k = 3$, entropy sums 4.43 vs. 4.64). For higher d , this method suffers from exponential complexity and diminishing distinguishability, which lead to intractability and numerical instability. So we applied a sampling strategy that confirms reliable classification, with inter-class gaps exceeding intra-class fluctuations by two orders of magnitude.

Exact Classification of MUBs for Prime Dimensions $d \leq 17$.— As shown in Table II, we compared the upper bounds on the amount of inequivalent MUBs classes obtained via the finite-operation transformation method with the lower bounds from the Shannon entropy criterion. Remarkably, for all $d \leq 17$, the two bounds coincide exactly, yielding the first complete classification of inequivalent MUBs subsets in this regime. Moreover, our upper bounds results exhibit strong consistency with the lower bounds obtained from the robustness of incompatible measurements criterion (covering partial

cases with $d \leq 31$ and $3 \leq k \leq 8$) [41], with only one exception in all $d \leq 17$: in the case $d = 17, k = 8$, our method gives 27 classes (matching the Shannon entropy criterion) while robustness yields 23. This discrepancy highlights a key advantage of our approach: entropy- and robustness-based criteria are sensitive to numerical precision and may merge nearly indistinguishable classes (with entropy differences < 0.01), whereas our transformation-based method remains virtually unaffected by such errors. Detailed classifications are provided in Sec. VII of SM. These features make our approach particularly powerful for reliably distinguishing inequivalent MUBs subsets, especially in higher dimensions.

In higher dimensions ($d \geq 19$), we provided upper bounds on the amount of inequivalent MUBs subsets up to $d = 37$ (Table II). When the subset size k is relatively small (e.g., $k \leq 5$), these upper bounds exactly coincide with the lower bounds derived from the robustness of incompatible measurements criterion. This congruence signifies that the exact amount of inequivalent MUBs subsets is precisely determined for these low-order subsets. However, for larger values of k , some discrepancies emerge between our derived upper bounds and the known lower bounds. In these instances, the exact amount of inequivalent classes is strictly constrained between our calculated upper bounds and the previously established lower bounds.

Distinguishing Inequivalent MUBs Subsets in Prime-Power Dimensions.— This finite-operation MUBs classification method can be extended to Hilbert spaces of prime-power dimension $d = p^n$ [4, 57] to explore their MUBs subset inequivalence classes. In prime-power dimensions, constructing the candidate set of unitary transformations requires the inclusion of equivalent MUBs generated by column-permutation operations P ($PP^T = I$), specifically $M_x P$, which reorder

TABLE II. A comparison of the amount of inequivalence classes generated by various MUBs subsets classification methods. The **blue** values represent the amount of classes identified using the proposed finite equivalence operational method. The **purple** values show the amount of classes derived from the Shannon entropy criterion. The **cyan** values indicate the amount of classes obtained using the robustness of incompatible measurements. Crucially, for dimensions up to $d \leq 17$, the classification results from the finite operation method and the entropy criterion exactly coincide, thereby establishing the precise equivalence classification of MUBs subsets in this range.

$k \backslash d$	5	7	8	9	11	13	17	19	23	29	31	37
3	2 2 2	1 1 1	1 1 1	2 2 2	1 1 1	2 2 2	2 2 2	1 1 1	1 1	2 2	1 1	2
4	1 1 1	2 2 2	1 1 1	3 3 3	2 2 2	4 4 4	4 4 4	4 4 4	4 4	6 6	6 6	9
5	1 1 1	1 1 1	1 1 1	3 3 3	2 2 2	5 5 5	8 8 8	5 5 5	6 6	19 19	11 11	29
6	1 1 1	1 1 1	1 1 1	3 3 3	4 4 4	7 7 7	15 15 15	13 13 13	22 22	68 67	51 50	140
7		1 1 1	1 1 1	2 2 2	2 2 2	10 10 10	20 20 20	18 18 18	36 32	194 145	132 92	552
8		1 1 1	1 1 1	1 1 1	2 2 2	7 7 7	27 27 23	31 22	83 35	531 ?	415 ?	2044
9			1 1	1 1	1 1	5 5	34 34	33	125	1255	992	6624
10				1 1	1 1	4 4	27 27	44	196	2576	2318	
11					1 1	2 2	20 20	33	227	4628		
12					1 1	1 1	15 15	31	268			
13						1 1	8 8	18	227			
14						1 1	4 4	13	196			
15							2 2	5	125			
16							1 1	4	83			
17							1 1	1	36			
18							1 1	1	22			
19								1	6			
20								1	5			

the column vectors within each basis. We rigorously demonstrate that it suffices to analyze the transformation paths of $M_d P$ (i.e., the action of the permutation matrix P itself) to uniquely determine all equivalent transformations $M_x P$ (Sec. VI of SM). Therefore, the extended set of unitary transformations is defined as:

$$\mathcal{U}_{\text{Efinite}} = \{U \in \mathcal{U}_{\text{finite}}\} \cup \{P \in \mathcal{P}_d\}, \quad (3)$$

where $\mathcal{P}_d$ is the set of column permutations that preserve the complete transformation property. While $d!$ permutations exist in total, only those maintaining MUBs completeness are included (constructive method in Sec. V of SM). Notably, in prime dimensions ($d = p$), the inclusion of column permutations does not fundamentally alter the classification, simplifying $\mathcal{U}_{\text{Efinite}}$ back to $\mathcal{U}_{\text{finite}}$. Finally, the full finite-operation set, composed of the extended unitary transformations $\mathcal{U}_{\text{Efinite}}$ and complex conjugation, allows us to apply the complete classification method to study inequivalent MUBs subsets in all prime-power dimensions.

We applied the extended finite-operation classification method to the prime-power dimensions ($d = p^n$), based on the maximal complete MUBs constructions of Ioannou *et al.* [58]. For $d = 8$ ($p = 2, n = 3$) with 9 maximal MUBs, $168 = 3 \times 8 \times 7$ column permutations preserve completeness, and all k -base subsets form a single equivalence class (Table II), consistent with lower bounds from Shannon entropy and robustness of incompatible measurements. In $d = 9$ ($p = 3, n = 2$), our upper bounds exactly match these lower bounds, e.g., $k = 4$ yields three inequivalent classes. We fur-

ther extended the study to $d = 16$ (Sec. VII of SM), demonstrating the broad applicability and reliability of our method in prime-power hilbert spaces.

Resource Consumption Analysis.— Evaluating the effectiveness of MUBs subset classification naturally requires considering its computational cost. Here, we compare the three methods by analyzing the resources needed to distinguish inequivalence classes of k -MUBs subsets. A detailed discussion is provided in Sec. VIII of the SM. Firstly, the finite-operation method reduces the classification of MUBs subsets to a discrete transformation-matching problem. A $[(d+2) \times (d+1)]$ transformation table, built from the actions of $\mathcal{U}_{\text{finite}}$ and complex conjugation, can be generated efficiently and quickly. For each k -subset check, extracting and normalizing the corresponding columns requires a complexity of $\mathcal{O}((d+2) k \log k)$. Since this procedure must be repeated $\binom{d+1}{k}$ times, the total complexity is

$$T_U = \binom{d+1}{k} \cdot (d+2) \cdot k \log k \cdot \mathcal{O}(d, \text{other}). \quad (4)$$

where $\mathcal{O}(d, \text{other})$ denotes the fixed overhead associated with extracting and storing equivalent subsets. Secondly, the Shannon-entropy-based method, in principle, requires exploring the entire pure states in the Hilbert space to determine the minimal entropy sum. For each k -subset check, a d -dimensional pure state $|\psi\rangle$ can be parameterized by $2d - 1$ parameters ($d - 1$ amplitudes $\alpha_m \in [-\pi, \pi]$ and d phases $\phi_n \in [0, 2\pi]$), and if each parameter is discretized into s points, a total of s^{2d-1} states must be evaluated. Conse-

quently, the total complexity of this method can be easily characterized as

$$T_S = \binom{d+1}{k} \cdot s^{2d-1} \cdot \mathcal{O}(k, d, \text{other}). \quad (5)$$

where $\mathcal{O}(k, d, \text{other})$ depend on the cost of single measurement and entropy calculation. Thirdly, the classification based on the robustness of measurement incompatibility requires solving a semidefinite program (SDP) for each of the $\binom{d+1}{k}$ subsets. For a given subset, the SDP involves d^k classical strategies, $(d^2 - 1)$ variables per operator G_λ , and on the order of dk constraints, with parameter scans contributing only subdominant overhead. The resulting total complexity scales as

$$T_R = \binom{d+1}{k} \cdot d^k \cdot (d^2 - 1) \cdot d \cdot k \cdot \mathcal{O}(s, \lambda, \text{other}). \quad (6)$$

where $\mathcal{O}(s, \lambda, \text{other})$ accounts for the SDP-solving overhead.

As shown in Fig. 2, the computational complexities of the three classification methods can be compared intuitively. For a fixed subset size k , the figure illustrates how T_S , T_R , and T_U scale with the dimension d . The Shannon-entropy-based method requires exponential sampling ($T_S \propto s^{2d-1}$), leading to an exponential increase in complexity with d . The classification based on the robustness of measurement incompatibility similarly exhibits exponential growth with d and k , due to the need to solve a large semidefinite program (SDP) for each subset. In contrast, the finite-operation method scales only linearly with d , avoiding high-dimensional numerical optimization and significantly improving computational efficiency.

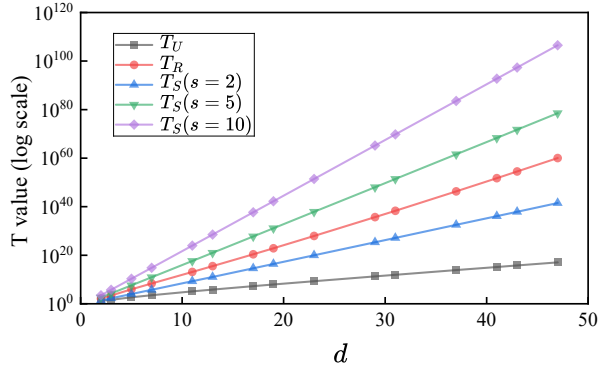


FIG. 2. Comparison of computational complexity rates as a function of the dimension d for the classification of MUB subsets with subset size $k = (d + 1)/2$, based on Shannon entropy, robustness of measurement incompatibility and finite equivalence operations, under different sampling densities $s = 2, 5, 10$.

In Sec. IX of SM, we further evaluate computational time of the other MUBs subsets classification approaches—including numerical optimization based on robustness of incompatible measurements, steering robustness, QRAC accuracy, and diamond distance. It is shown that the finite-operation method

drastically reduces both computation time and cost while preserving accuracy. For instance, for $d = 31, k = 8$, competing methods approach their processing limits, whereas our method completes full classification in under three minutes.

Conclusions and Discussions.— In conclusion, we have introduced a robust and resource-efficient finite-operation framework for the structural classification of MUBs subsets. For arbitrary sets of k MUBs in any prime dimension d , this method yields a universal analytical upper bound for the amount of MUBs equivalence classes. By applying this method through simple iterations, we further obtain tighter classification upper bounds for prime dimensions $d \leq 37$. Crucially, comparing these upper bounds with existing lower bounds, we successfully determine the exact inequivalence classes for all MUBs subsets in dimensions $d \leq 17$. Furthermore, the framework's extension to prime-power dimensions and its proven computational efficiency mark a significant step forward. This systematic classification provides robust theoretical and algorithmic support essential for high-dimensional quantum resource certification and measurement design. In addition, the framework can be further tightened in prime-power dimensions by incorporating an overall global phase into the unitary operation $\mathcal{U}$. More broadly, the classification method developed here is directly useful for a variety of high-dimensional quantum information tasks, such as quantum randomness generation, quantum key distribution, multi-party cryptography, entanglement witnessing, quantum metrology, etc.

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